TRABAJO FIN DE GRADO

SIMULACIÓN NUMÉRICA DE LA ECUACIÓN DE SCHRÖDINGER EN 2D

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Dedicado a mi madre,
sin cuyo esfuerzo ni
sacrificio me hubiese
resultado imposible
cursar la carrera.

RESUMEN

La transición entre el siglo XX y XXI, con el vertiginoso avance en el campo de las nuevas tecnologías, en especial en el de informática y computación, ha permitido realizar simulaciones cada vez más compicadas, con un gasto de tiempo y recursos inferior. Simulaciones para las que no hacía tanto tiempo se necesitaban los ordenadores más potentes de la época, en la actualidad pueden ser llevados a cabo incluso en el ámbito académico.

Una de aquellas simulaciones, tratada en el presente trabajo, se centra en reproducir, mediante la ayuda de los métodos numéricos, el comportamiento de una partícula subatómica no relativista, descrita por la ecuación de Schrödinger. Cabe destacar que, debido a la incertidumbre de Heisenberg, dicha ecuación es, junto con la mecánica matricial y la integral de caminos, una de las maneras de describir el estado de una partítica en mecánica cuántica. Así, en el capítulo primero nos vamos a centrar en el sentido físico de dicha ecuación y de su obtención matemática, así como trataremos de una forma breve algunos fenómenos en los que tiene alguna influencia.

Antes de empezar la simulación, tenemos que describir los métodos y técnicas empleadas. En el capítulo 2 pondremos nuestra atención en la parte numérica, explicando cómo se ha conseguido transformar una EDP en una EDO para poder llavar a cabo la simulación en el tiempo. A parte, también se introdujo un apartado sobre la solución analítica, para posteriormente poder hacer una comparación con los resultados numéricos obtenidos del método elegido.

La parte unidimensional, tanto el desarrollo del código como su verificación, así como la interpretación de los datos obtenidos, se estudian en el Capítulo 3. También veremos la influencia de los parámetros de la barrera en el coeficiente de transmisión para el efecto túnel.

El núcleo del trabajo, aquel que trata de la simulación en un espacio bidimensional, ocupa el capítulo 4. Aquí se explican los pasos hasta llegar a la simulación del experimento de Young, aquel que puede interpretarse como uno de los argumentos de la dualidad onda-corpúsculo. Al emplear la ecuación de Schrödinger, ya se sobreentiende que se trata de una partícula (por contener la masa m en su forma general). Tras pasar la barrera, muestra el fenómeno de difracción, una característica puramente ondulatoria.

Por último, en el quinto capítulo, hablaremos brevemente de los posibles trabajos que pudiesen desarrollarse a partir del presente, tales como aumentar el número de partículas, cada cual interactuando con las demás, o modificar el Hamiltoniano e intentar desarrollar la ecuación de Dirac para el movimiento de las partículas relativistas.

ABSTRACT

The transition of the XX and XXI centuries, with a vertiginous advance in new technologies field, especially in the informatics and computational ones, has permitted to make simulations each time more complicated, with a less spending of time and resources. Simulations for which not too long ago the most powerful computers of the time were needed, nowadays can be done even in an academic ambit.

One of those simulations, treated in the present work, is focused on reproducing, with the help of the numerical methods, the behavior of a non-relativistic subatomic particle, described by the Schrödinger equation. It worth to distinguish that due to the Heisenberg uncertainty principle, this equation is, along with the matrix mechanics and the path integral formulation, a manner of describing a state of a particle in the quantum mechanics. Thus, in the first chapter we are going to center in the physical meaning of this equation and its mathematical obtainment, as well as we are going to treat briefly some phenomenon upon which it has some influence.

Before starting the simulation, we have to describe the employed methods and technics. In the Chapter 2 we will center our attention in the numerical part, explaining how we have managed to transform a PDE into an ODE to carry out the time simulation. Apart, a paragraph about the analytic solution has been introduced, for the further comparison with the numerical results gotten from the chosen method.

The one dimensional part, both the script development and its verification, as well as the interpretation of the obtained results, are studied in the Chapter 3. We will also search for the influence of the barrier parameters on the transmission quotient for the tunnel effect.

The nucleus of the work, the one which is about the two dimensional simulation, occupies the Chapter 4. Here, steps which lead us to Young's experiment simulation are explained; the experiment which serves as an argument of the wave-particle duality. Once we use the Schrödinger equation, it is being understood that it is a particle (by containing the mass m in its general form). After going through the barrier, it shows the diffraction phenomenon, a purely wave-like characteristic.

Finally, in the fifth chapter, we will talk briefly about the potential works that could be developed using some information of the present one, such as increasing the number of particles, each one interacting with the rest, o modifying the Hamiltonian and trying to develop the Dirac equation for the relativistic particles motion.

CHAPTER 1.INTRODUCTION

1.1. PURPOSES OF THE PRESENT WORK

The complexity of the quantum world is so huge, that researches often try to search for some analogies between the quantum physics and some classical branches of science, being acoustics one of the most relevant [1]. The development of the informatics has supposed also a huge step toward comprehending some quantum phenomenon. In the present work, one of the final goals consists in simulating a double slit experiment, plotting out the diffraction behavior of a material subatomic particle with mass m using the Schrödinger equation, as well as some other phenomenon worth to be studied.

1.2. BRIEF HISTORICAL INTRODUCTION

At the beginning of the XX century, physicists have not yet been able to give a clear answer to the dual behavior (wave-particle) at a subatomic level. An equation, developed by an Austrian scientific Erwin Schrödinger back in 1925 [2] (it worth him a Nobel Prize in 1933) and complemented by Max Born during the next year (the probability of finding a particle in some spatial interval) is nowadays one of the columns of the modern quantum physics.

The equation establishes the wave function $\Psi(x,t)$, which describes and predicts the behavior of the system once the force which is acting upon the associated particle is known [3]. In other words, it is an equivalent of the second Newton law in quantum mechanics [2] [4]. In classical mechanics, knowing both the position and the momentum of a particle, we are able to calculate its motion in the future; nevertheless, in quantum mechanics, due to the Heisenberg uncertainty principle, we cannot know both at the same time, so the wave function is used instead, allowing us to predict the movement of the particle and the probability of finding it in some region, once some initial distribution is given, as well as its mass and the voltage in the space where the motion occurs.

It has plenty of uses both in physics and in chemistry, for example quantum computing or scanning tunneling microscope as the most remarkable ones. It also allows to explain a lot of natural phenomenon, such as the alpha-decay [5] [6], the structure of the atoms (for example, the hydrogen atom), and the production of unique line spectrum by atoms [4].

1.3. THE DEVELOPMENT OF THE THEORY AND TIME DEPENDENT SCHRÖDINGER EQUATION

Due to the fact that it is an equation which correctly predicts the results which can be verified by some kind of experiments, not being an equation developed from the experimental information, Schrödinger equation is therefore a postulate [2] [3] [6].

In order to be able to study it, we begin by assuming the following approaches [6]:

1) Creation and destruction of the material particles are assumed not to take place.
2) All material particles are moving with enough low speed so we may consider their movement as a “non-relativistic” one. The Dirac equation is an extension of the Schrödinger theory applied to “relativistic” particles (those whose velocities are next to the light speed) [2].

Besides, the wave equation has to be consistent with the following assumptions [3]:

1) De Broglie-Einstein postulate:
   λ=h/p and ν=E/h
2) The energy conservation
   E=p^2/2m+V
3) It has to be lineal.
4) If the voltage suffers no changes during the particle motion (F=0), the solution of the differential equation has the form of a sinusoidal travelling wave with a constant frequency. This fact is used below as one possible manner to prove the validity of the numerical simulation.

After the mathematical development taking into account the assumptions explained above, Schrödinger has obtained the following expression:

$$i\hbar\frac{\delta\Psi(r,t)}{\delta t}=H\Psi(r,t) \tag{1.1}$$

Being H the Hamiltonian operator (includes the total energy of the system). For a single particle the Hamiltonian becomes [1],[2],[33]:

$$H=-\frac{\hbar^2}{2m}\nabla^2+V(r)$$

So Schrödinger Equation is therefore a Partial Differential Equation (PDE), with both time and spatial dependences:

$$i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t}=-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r},t)+V(\vec{r})\Psi(\vec{r},t) \tag{1.2}$$

We must notice that almost in all cases the voltage has no time dependence, so it can be written as V(r).

Among the properties of any wave function we must notice the following ones [3] [6]:

1) It has to be continuous and unique at each point of space and for every instant of time.
2) Its first derivative has to be continuous and unique at each point of space and for every instant of time.
3) It has to be normalized, meaning that its probability distribution has to be finite.

There can also be traced some analogy between the classical conservation of energy and the Schrödinger equation, as the time derivative is equivalent to the total energy of the system, and -iħ∇ is the momentum in quantum mechanics (and therefore -$\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r},t)$ is equivalent to the classical expression for the kinetic energy $\frac{p^2}{2m}$)

1.4. SCHRÖDINGER TIME INDEPENDENT EQUATION [3]

Among the techniques used to solve the PDE, the separation of variables method is one of the most useful. This method transforms an equation which initially was depending on two variables (time and space), into a product of two equations, one determined by time and the other by space parameters, so the final solution has the following form:

$$\Psi(\vec{r},t)=\psi(\vec{r})\varphi(t)$$

Where $\Psi(\vec{r},t)$ is Schrödinger Time Dependent Equation; $\psi(t)$ is the time parameter; and $\varphi(\vec{r})$ is the wave function without time dependence obtained from Schrödinger Time Independent Equation.

Taking into account the classical wave equation, our solution has to satisfy the following expression:

$$\psi(\vec{r},t)=A\sin(k\vec{r}-wt)+B\cos(k\vec{r}-wt) \quad (1.3)$$

As we want a solution that does not depend on time (t=0):

$$\psi(\vec{r})=A\sin(k\vec{r})+B\cos(k\vec{r}) \quad (1.4)$$

with:

$$k=\frac{2\pi}{\lambda}=\frac{2\pi p}{h}=\frac{p}{h/2\pi}=\frac{p}{\hbar}$$

$p=k\hbar$

As it has to satisfy the law of conservation of energy:

$$E=K+V=\frac{1}{2}mv^2+V=\frac{1}{2}\frac{p^2}{m}+V=\frac{1}{2}\frac{k^2\hbar^2}{m}+V \quad (1.5)$$

where:

E=total energy

K=kinetic energy

V=potential energy

Taking a second derivative of (1.4):

$$\nabla^2\psi=-k^2\psi(r) \quad (1.6)$$

and multiplying both sides by $-\hbar^2/2m$

$$\frac{-\hbar}{2m}\nabla^2\psi=\frac{-\hbar^2k^2}{2m}\psi \quad (1.7)$$

On the other hand, multiplying (1.5) by ψ and taking the kinetic energy term:

$$\frac{\hbar^2 k^2}{2m}\psi=(E-V)\psi \quad (1.8)$$

Combining (1.7) and (1.8), the result is the following expression:

$$\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r})=[V(\vec{r})-E]\cdot\psi(\vec{r}) \quad (1.9)$$

called Schrödinger Time Independent Equation, with the time parameter as

$$\varphi(t)=e^{-iEt/\hbar} \quad (1.10)$$

being:
ħ: reduced Planck constant (also called Dirac constant)
E: total energy available for the particle
m: particle mass

Therefore, the main difficulty lies on being able to solve the Time Independent Equation, in order to have the time evolution of the wave.

1.5. PROBABILITY STATISTICS OF SCHRÖDINGER EQUATION [3] [6] [2]

The probability of finding a particle in a determined space region for a concrete time is proportional (demonstrated by Max Born) to the square of the wave amplitude:

$$P(\vec{r},t)=|\Psi(\vec{r},t)|^2 \quad (1.11a)$$

or, being a complex function, as:

$$P(\vec{r},t)=\Psi^*(\vec{r},t)\Psi(\vec{r},t) \quad (1.11b)$$

where $\Psi^*(\vec{r},t)$ is the conjugate of the wave $\Psi(\vec{r},t)$.

1.6. QUANTUM TUNNELING AND THE THEORY OF ALPHA DECAY [5] [6]

The dual nature of the microscopic particle, which mathematically results in a complex wave equation, leads to a particularly interesting phenomenon called quantum tunneling [6][7]. It consists in a possibility of a particle to overstep a voltage barrier even if its total energy is less than then the voltage value. It is an impossible phenomenon in classical physics, for which the particle would bounce back keeping its energy (if there are no losses in the crash). Inside a potential region, the wave function begins to decay exponentially, so it will emerge on the other side of the barrier with smaller amplitude. The main parameters to find out which part of the wave is reflected backwards, and which is transmitted through the barrier are the difference between the barrier voltage and the energy of the particle, the width of the barrier and the particle mass.

The quantum tunneling is extremely important in the knowledge of the radioactive decay, especially alpha decay. The alpha decay theory, developed by George Gamow, explains how the radioactive atomic nucleus throws out an alpha particle, decreasing its mass number by 4 units, and its atomic number by 2 (or what is the same, losing two neutrons and two protons) and emitting some energy.

This theory is based on the supposition that the alpha particle is being trapped in a potential well generated by the nucleus. The particle is constantly bouncing from one side to another, and although its energy is lower than the barrier, with each crash it has a tiny probability of 'tunneling' through it and escape the nucleus. Gamow has also determined the relation between the energy of the α-particle (which typically lies in the range of 4-10 MeV) and the half-life of the decay: the higher is the energy of the α-particle, the lower is the half-life.

CHAPTER 2. METHODS USED IN THE SIMULATION

2.1 INTRODUCTION

Due to the fact that Schrödinger equation is a Partial Differential Equation (PDE), in most cases it is very laborious (or even impossible) to find an analytical solution of the wave. For such purpose, and taking advantage of computing power, numerical methods which are able to solve almost every problem are often used.

After obtaining some numerical results, we have to confirm their validity; in that case we should compare a numerical method with the analytical one, or compare two numerical methods among them. Some other comparisons are used, each one explained in the appropriate case.

Moreover, we tried to develop two numerical methods to solve the initial problem, so that each one is compared to the analytical solution, and then each other. In this way, we should be able to verify the truthfulness of both methods and compare which one has less error and takes less time to simulate. The chosen ones were the Method of Lines (MoL) and the Leapfrog method, both based on the discretization. There are some other possibilities such as using the Hamiltonian operator. But due to the lack of time, this purpose has not been completed, and we have centered our efforts basically on the MoL.

2.2 METHOD OF LINES (MOL)

This method is based on the discretization of all but one dimension (in our case it will be the time dimension) [8][9][10]. Developing the Taylor series around each point, we obtain the following expression for the second space derivative in x axis [9][10]:

$$\frac{\delta^2\Psi}{\delta x^2}=\frac{\Psi(x-\Delta x,t)+\Psi(x+\Delta x,t)-2\Psi(x,t)}{\Delta x^2} \tag{2.1}$$

where Δx is the distance between two consecutive points of the space grid. One can notice that to know the value of any point in the following instant, it is necessary to know the values of the wave at the surrounding points in the previous time period.

Once the spatial derivative is discretized, PDE becomes an ODE, so MATLAB operators such as ODE45 or ODE23s might be used to solve the space grid for each instant of time [11].

To start the iteration, the initial form of the wave has to be known, as well as the boundary conditions, that in our case are of the Dirichlet form [12] and equal to zero (that is, the wave is confined in some kind of "box", outside of which the wave does not exist). On the other hand, the initial Gaussian wave packet has the next dispersive form:

$$\Psi(x,t=0)=A\cdot\exp\left(-\frac{x-x_0}{2\cdot\sigma^2}\right) \tag{2.2}$$

with:

x_0=center of the wave packet

σ=diameter of the initial wave packet

A=constant result of the normalization

2.3. LEAPFROG METHOD [10] [13] [14] [15]

As the wave is a complex function, it can be divided into two parts, a real one (written as ReΨ) and an imaginary one (ImΨ):

$$\Psi=Re\Psi+i\cdot Im\Psi \tag{2.3}$$

Introducing this expression into the Schrödinger time dependent equation, and taking the real terms on the one hand, and those which depend on the imaginary number i on the other, we obtain two equations:

$$\frac{\delta Im\Psi}{\delta t}=\frac{1}{2}\frac{\delta^2 Re\Psi}{\delta x^2}-V(x)Re\Psi \tag{2.4a}$$

and

$$\frac{\delta Re\Psi}{\delta t}=-\frac{1}{2}\frac{\delta^2 Im\Psi}{\delta x^2}+V(x)Im\Psi \tag{2.4b}$$

Taking the finite differences in the expressions above, both for time and space parameters, and designing $s=\frac{\Delta t}{(\Delta x)^2}$:

$$Im\Psi(x,t+\Delta t)=Im\Psi(x,t-\Delta t)+sRe\Psi(x+\Delta x,t)+s\cdot Re\Psi(x-\Delta x,t)-2\cdot(s+\Delta t\cdot V(x))\cdot Re\Psi(x,t+\Delta t) \tag{2.5a}$$

Before discretizing the equation (2.3), we can observe that there is some kind of "alternant" feature referred to the time, both for the real and the imaginary parts. If the real part is evaluated for time t, then the imaginary part should be calculated for previous or later intervals of times. Following this alternant model, the discretization for (2.3) is:

$$Re\Psi(x,t+2\cdot\Delta t)=Re\Psi(x,t)-s\cdot Im\Psi(x+\Delta x,t+\Delta t)-s\cdot Im\Psi(x-\Delta x,t+\Delta t)+2\cdot(s+\Delta t\cdot V(x))\cdot Im\Psi(x,t+\Delta t) \tag{2.5b}$$

This form gives us some trouble, cause to know the wave value in the next time step, we must know not only the value of a current time step, but also in a previous one, thing that is clearly impossible for the first iteration. To avoid this inconvenience, we just assume that at the beginning the values at t=-Δt are the same as at t=0.

The second difficulty of this method lies on the fact that in each time interval we can only obtain the improved value of only one part, not both at the same time. Therefore, we adopt the criterion of evaluating the imaginary part of the wave at the odd time intervals, while the real part is updated during the real time steps.

Finally, we obtain the following expressions (m refers to the time steps, while j refers to the spatial grid):

$$Im\Psi_j^m=Im\Psi_j^{m-2}+s\cdot Re\Psi_{j+1}^{m-1}+s\cdot Re\Psi_{j-1}^{m-1}-2\cdot(s+V_j\cdot\Delta t)\cdot Re\Psi_j^{m-1} \quad \text{if m=odd} \tag{2.6a}$$

And

$$Re\Psi_j^m=Re\Psi_j^{m-2}-s\cdot Im\Psi_{j+1}^{m-1}-s\cdot Im\Psi_{j-1}^{m-1}+2\cdot(s+V_j\cdot\Delta t)\cdot Im\Psi_j^{m-1} \quad \text{if m=even} \tag{2.6b}$$

In the same way, the statistical probability of the wave also depends whether the time step is odd or even:

$$|\Psi|^2=(Re\Psi_j^m)^2+\mathrm{Im}\Psi_j^{m+1}\cdot\mathrm{Im}\Psi_j^{m-1} \qquad \text{if m=even} \qquad (2.7a)$$

And

$$|\Psi|^2=\mathrm{Re}\Psi_j^{m+1}\cdot\mathrm{Re}\Psi_j^{m-1}+(Im\Psi_j^m)^2 \qquad \text{if m=odd} \qquad (2.7b)$$

2.4. ANALYTICAL SOLUTION [3] [16]

As we have already seen before, it is possible to obtain the time-dependent wave function only by multiplying its time-independent form by a time parameter. Therefore, the main difficulty lies in searching for such time-independent wave functions that can solve our initial problem.

$$\Psi(\vec{r},t)=\psi(\vec{r})\cdot\varphi(t)$$

The best way to get a solution is by using the Sturm-Liouville theory. To proceed with this method, it is necessary to delimitate the space region where the particle is going to move. For such purpose Dirichlet boundary conditions are imposed.

Solving the Sturm-Liouville problem with a fixed voltage distribution, it can be noticed that in order to have an exact solution one cannot take any value of energy E. Moreover, the energy value which gives us an exact wave function is called eigenvalue (E_n), meanwhile the wave function is called eigenfunction (Ψ_n). An eigenvalue gives us only one eigenfunction, and also vice versa.

Due to the fact that Schrödinger equation is a linear differential equation for wave function Ψ, we can use one property that helps us in a further analytical solution: the superposition principle. It establishes that a particle may partially exist in all theoretically possible states at the same time, but when it is measured the result corresponds only to one possible configuration. This principle allows us to consider a wave function for any given energy value as the linear combination of two or more eigenfunctions with their correspondent eigenvalues:

$$\Psi(\vec{r},t)=\sum_{n=1}^{\infty} c_n\cdot\psi_n(\vec{r})\cdot e^{-iE_nt/\hbar} \qquad (2.8)$$

where n corresponds to the order of eigenvalue from smaller to bigger.

CHAPTER 3. 1D SCHRÖDINGER EQUATION

3.1 NUMERICAL METHOD

As we have yet seen, first of all we proceed by calculating the numerical solution by MoL, for its further comparison with the analytical solution to validate the numerical technique.

In order to simplify the 1D case, we should obtain the dimensionless form of the Schrödinger equation. For such purpose, we begin by dividing all the Schrödinger equation (1.1), given only in one dimension, by the available energy of the particle, E, and the imaginary number, i:

$$\frac{\hbar}{E}\frac{\partial\Psi(x,t)}{\partial t}=\frac{i\hbar^2}{2mE}\cdot\frac{\partial^2\Psi(x,t)}{\partial x^2}-i\frac{V}{E}\Psi(x,t) \tag{3.1}$$

We continue by assigning the following dimensionless parameters:

$$\mathrm{T}=\frac{t_c E}{\hbar} \qquad \bar{x}=\frac{x_c}{L} \qquad \bar{\mathrm{U}}=\frac{V}{E}$$

Notice that the ratio between the height of the voltage barrier and the energy of the particle, called $\bar{\mathrm{U}}$, has a great influence in the quantum tunneling effect.

As a result, we obtain the following expression:

$$\frac{\partial\Psi(\bar{x},\mathrm{T})}{\partial\mathrm{T}}=\frac{i}{2}\frac{\hbar^2}{mEL^2}\cdot\frac{\partial^2\Psi(\bar{x},\mathrm{T})}{\partial\bar{x}^2}-i\bar{\mathrm{U}}\Psi(\bar{x},\mathrm{T}) \tag{3.2}$$

Being $\chi=\frac{\hbar^2}{mEL^2}$ another dimensionless parameter

Furthermore, let us look upon a wave packet being trapped in a space region with a constant voltage in all its dominion, that is, no change in the potential energy is taking place ($\bar{\mathrm{U}}=0$). Assigning also that $\chi=1$, the expression is reduced to:

$$\frac{\partial\Psi}{\partial\mathrm{T}}=\frac{i}{2}\frac{\partial^2\Psi}{\partial\ddot{\mathrm{x}}^2} \tag{3.3}$$

a form much easier to be solved by the analytical method.

The following step consists in discretizing the equation above with the help of (2.1):

$$\frac{\partial\Psi}{\partial\mathrm{T}}=\frac{i}{2}\cdot\frac{\Psi(\bar{x}-\Delta x,\mathrm{T})+\Psi(\bar{x}+\Delta x,\mathrm{T})-2\Psi(\bar{x},\mathrm{T})}{\Delta\bar{x}^2}$$

Moreover, we must impose some boundary conditions, a zero value in the borders, and describe the initial condition for the wave, using for such purpose a Gaussian wave packet, with its general dispersive form (spreading equally in all space directions) given by:

$$\Psi(\bar{x},\mathrm{T}=0)=\mathrm{A}\cdot\exp\left(\frac{-(\bar{x}-\bar{x}_0)^2}{2\sigma^2}\right) \tag{3.4}$$

With:

A= normalization constant which makes the probability of finding a particle in the space grid equal to 1

$\bar{x}_0$=center of the Gaussian wave packet

σ=a parameter describing the "initial diameter" of the wave packet, or how the probability is located around its center

3.2. ANALYTICAL METHOD

Now, once the normalization of the wave packet is done, solving the Sturm-Liouville problem [9],[18], we get that for a grid without any kind of changes in the voltage field, eigenfunctions and eigenvalues take the following form:

$$\varphi_n(x)=\sqrt{2}\sin(\frac{n\pi x}{L})$$

$$E_n=\frac{\pi^2\hbar^2}{2mL^2}n^2$$

Replacing these parameters into the superposition principle [9]:

$$\Psi(x,t)=\sum_{n=1}^{\infty} c_n\cdot\sqrt{2}\cdot\sin(\frac{n\pi x}{L})\cdot e^{-i\frac{\pi^2\hbar}{2mL^2}tn^2} \quad (3.5)$$

And using the dimensionless space and time parameters and the fact that $\frac{mL^2}{t^2}$=E, the following expression is obtained:

$$\Psi(\bar{x},T)=\sum_{n=1}^{\infty} c_n\cdot\sqrt{2}\cdot\sin(n\pi\bar{x})\cdot e^{-\frac{i}{2}(n\pi)^2 T} \quad (3.6)$$

Using the orthonarmality of the eigenfunction, with the initial form of the wave packet we integrate:

$$c_n=\int_0^1 \varphi_n(\bar{x})\cdot\Psi(\bar{x},0)d\bar{x} \quad (3.7)$$

We can easily get the values of the constants using the trapz function in MATLAB, to be finally able to obtain the complete analytical solution changing during the time.

3.3. COMPARISON BETWEEN THE METHODS

Once both analytical and numerical (by ode45) solutions are obtained, it is time to overlay the probability density to check the validity of the numerical method. The chosen instant is T=0.02.

After a successful comparison, the following plot is obtained for T=0.02:

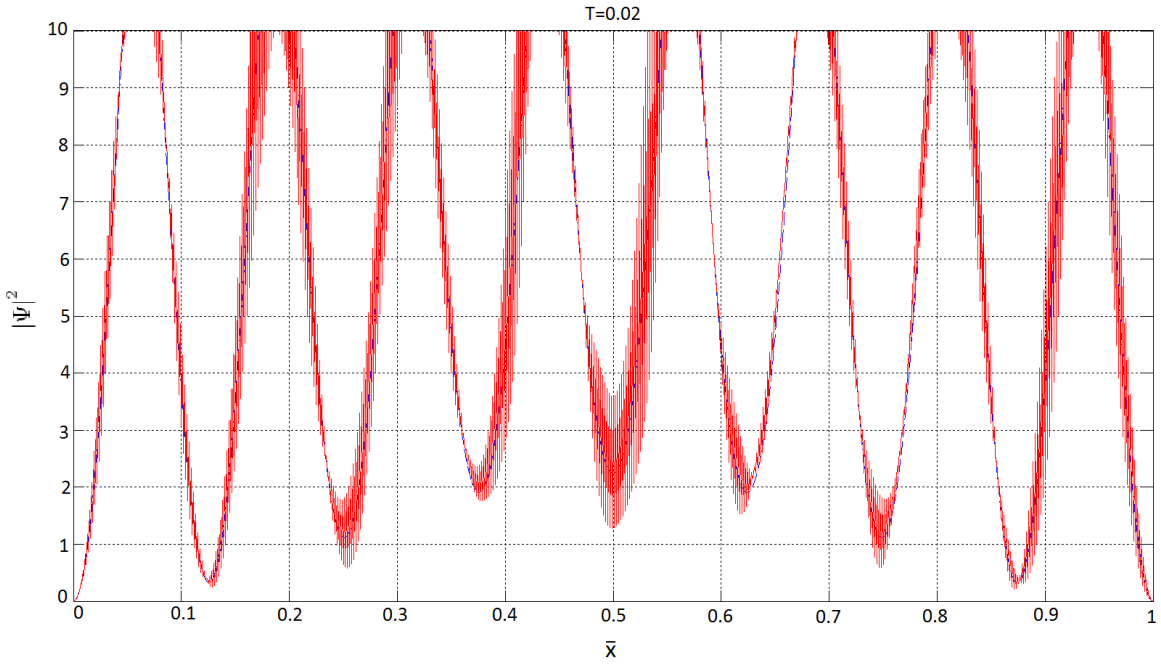


FIG 2.1. Comparison of the local wave probability at T=0.02 for both methods. In this case, numerical solution is designated by a red color, while the analytical one is painted in blue.

As we can see, there is some precision error caused by the numerical method, but in general terms it is quite valid. More accuracy is obtained if we use more points and the distance between them is smaller. 1000 points are used to compare the solutions.

3.4. NUMERICAL RESULTS

Now that the numerical simulation is proved, we can impose some barrier condition. In our first case, the chosen voltage barrier is 10000 times larger than the energy of the particle, and it is localized in $0.6<\bar{x}<0.7$. We must also prove whether if the probability of finding a particle in all spatial grid remains constant during the time, multiplying the wave probability in each interval by its length; prob=$|\Psi^2|\cdot d\bar{x}$. The running time T is equal to 0.005.

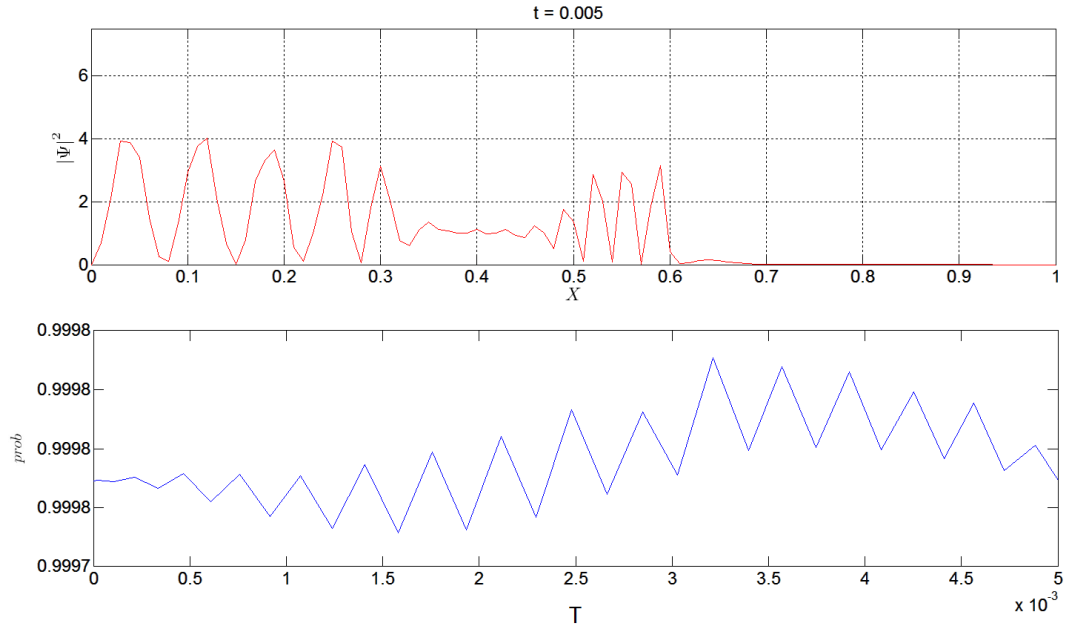


FIG 2.2. Above. Local wave probability at T=0.005. Below: the total probability at all space grid during the time. Ū=10000

As it can be observed, there is practically no wave which oversteps the barrier, so now we should change the ratio between the voltage and the energy of the particle in order to sight the results and get some conclusions (Ū=10). The barrier still remains in the same position.

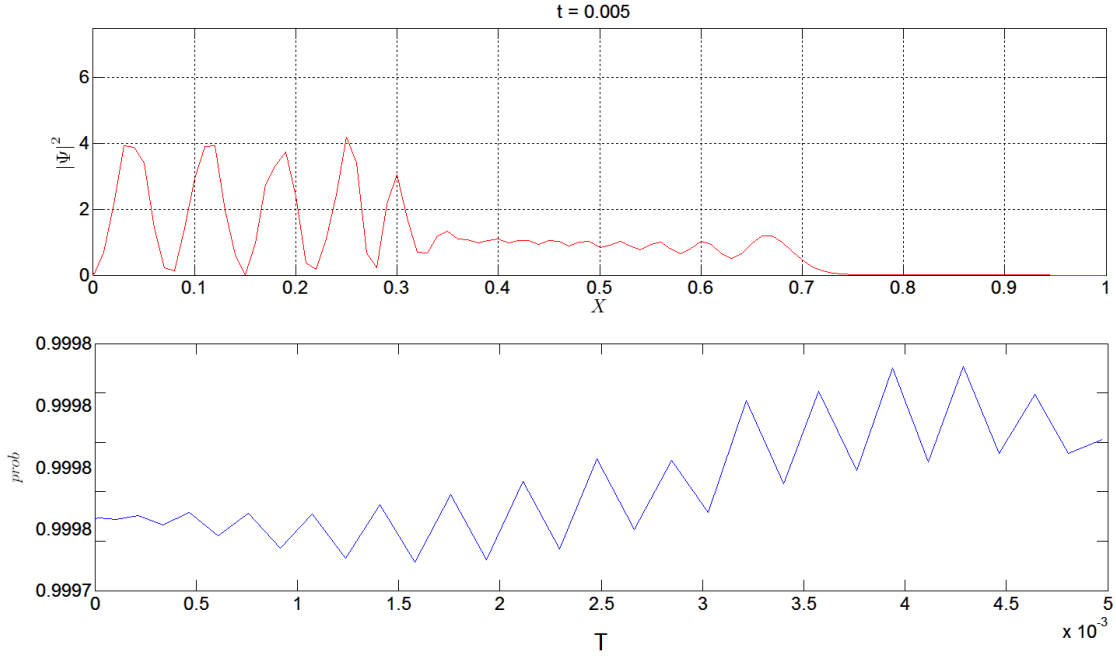


FIG 2.3. Above. Local wave probability at T=0.005. Below: the total probability at all space grid during the time. Ū=10

At low ratio values, the wave almost entirely comes over the barrier. One possible explanation to this phenomenon is the small thickness of obstacle, as the wave decreases exponentially inside the voltage.

Also in 1D we can easily plot both the imaginary and the real parts of the wave, the cause which makes possible the quantum tunneling.

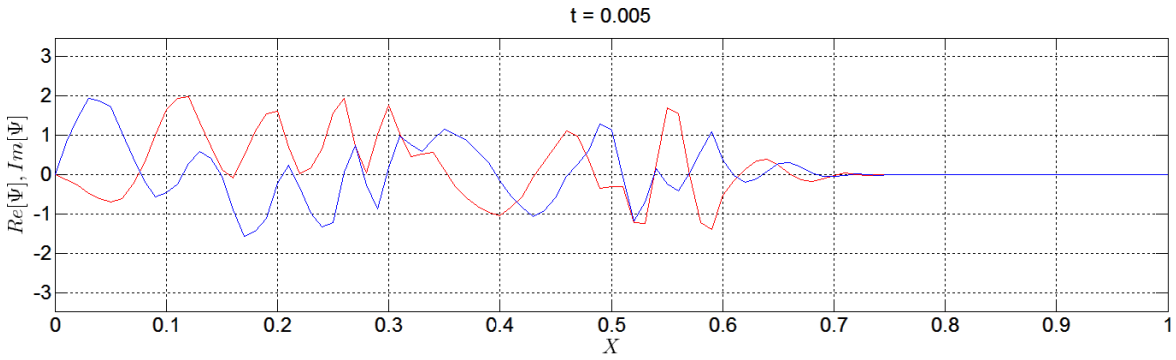


FIG 2.4. Real and imaginary components of the wave for the same period of time. The real part is represented in blue, meanwhile the imaginary one in red.

3.5. TRANSMISSION QUOTIENT

In this paragraph we are going to discuss the relation of the ratio ($\bar{U}$) and the width of the barrier (a), and the part of the wave which passes through it and emerges on the other side due to quantum tunneling effect. Let us start by describing a dimensionless space grid in one unique dimension (delimited by Dirichlet Boundary Conditions), with a potential barrier higher than the total amount of the energy of the particle. The wave associated to our particle initially has the form of Gaussian wave packet. We are going to describe a generic case, so parameters of the barrier and the wave are irrelevant. The only thing to mention is that we have chosen that the wall is located to the right of the wave. The grid is divided into three regions, the ones before, below and after the voltage barrier [17].

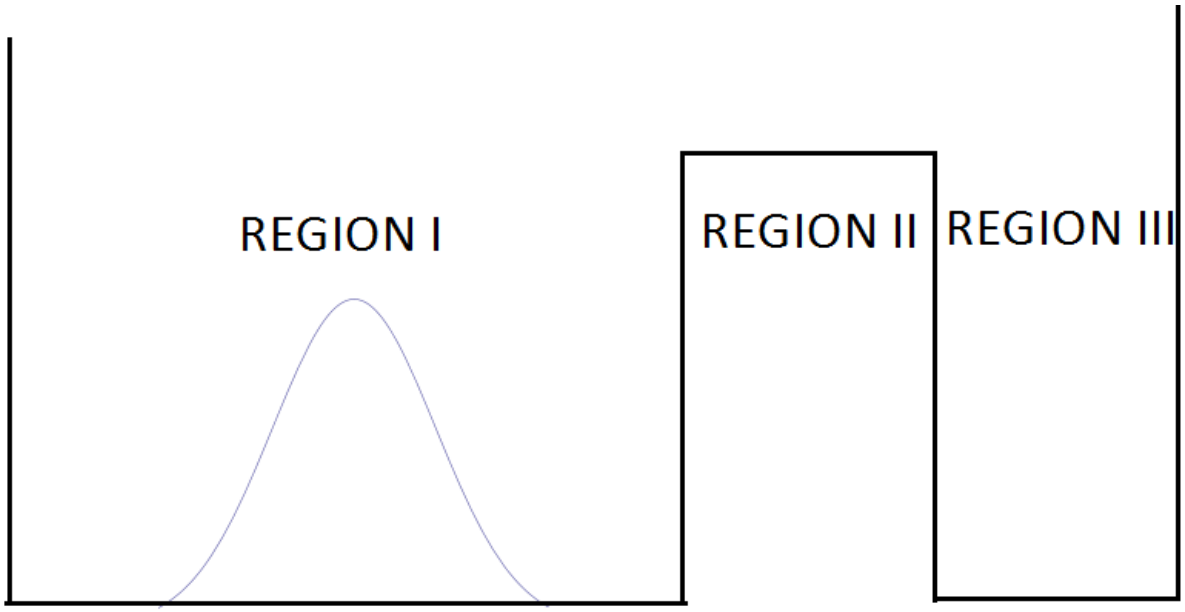


FIG 2.5. Voltage distribution.

The important thing to consider in this example is the Schrödinger time independent equation, because the order of magnitude of the wave which passes through the barrier is more or less the same during the time marching.

$$-\frac{\hbar^2}{2\cdot m}\frac{d^2\psi}{dx^2}=[V(x)-E]\cdot\psi(x)$$

Making it dimensionless:

$$\bar{x}=x/L \qquad \chi=\frac{E\cdot m\cdot L^2}{\hbar^2} \qquad \bar{U}=\frac{V(x)}{E}$$

We get:

$$-\frac{1}{2}\frac{d^2\psi}{d\bar{x}^2}=(\bar{U}-1)\cdot\psi(\bar{x}) \tag{3.8}$$

For the first region ($\bar{U}=0$), its general solution takes the form:

$$\psi_I=A\cdot\exp(i\cdot\sqrt{\chi}\cdot\bar{x})+B\cdot\exp(-i\cdot\sqrt{\chi}\cdot\bar{x}) \tag{3.9a}$$

The positive exponential is the responsible for the wave moving to the right, while the negative one produces a wave moving to the left.

In the region II, the one affected by the barrier, the solution form of time-independent equation is:

$$\psi_{II}=C\cdot\exp[i\cdot\sqrt{\chi}\cdot(\bar{U}-1)\cdot\bar{x}]+D\cdot\exp[i\cdot\sqrt{\chi}\cdot(\bar{U}-1)\cdot\bar{x}] \tag{3.9b}$$

In an analogous way, the general solution for the region III is (the constant E should be replaced by another letter to avoid possible misunderstanding with the energy of the particle, called E):

$$\psi_{III}=F\cdot\exp(i\cdot\sqrt{\chi}\cdot\ddot{x})+G\cdot\exp(-i\cdot\sqrt{\chi}\cdot\ddot{x}) \tag{3.9c}$$

Imposing the continuity both of the wave and of its first derivative at the beginning and at the end of barrier, and taking into account that once the wave has passed the obstacle, its movement continues only forward (G=0), we have got a system of 4 equations and 5 unknown constants. But we are able to obtain the relation between the quotients A and F, or what is the same, the relation between the wave that falls upon the voltage barrier, and that part which passes through and appears on the other side. It is better to operate with the probability, not with the wave itself. The square of the ratio between F and A is called transmission quotient, represented by the letter T [16][17]:

$$T=\left(\frac{F}{A}\right)^2$$

Operating, it gives us the following result:

$$T=\frac{1}{1+\frac{senh^2[\sqrt{2}\cdot\sqrt{\chi}\cdot\left(\frac{1}{\bar{U}}-1\right)\cdot\bar{a}]}{4\cdot\frac{1}{\bar{U}}\cdot(1-\frac{1}{\bar{U}})}} \tag{3.10}$$

Where ā is the dimensionless width of the barrier ā=a/L. We can also suppose that the constant χ is practically the unity. For the cases we have been studying, the barrier occupies the tenth part of the entire grid, so ā=0.1. Now, let us replace the constant Ū by its numerical value to regard whether if the obtained computer results are likely to be certain. For Ū=10000, the obtained transmission quotient is about 0.0195, meaning that there is almost 2% of probability for a certain wave to pass the barrier which is 10000 as high as the whole amount of energy of the particle associated to the wave. Decreasing the ratio Ū, for example to Ū=1000, T=0.1659. For such configuration, the "quantum tunneling" is well observed, as the part overstepped through the barrier is comparable in the order of magnitude to the one reflected. And finally, for Ū=10, the transmission is T=0.9567, with practically no attenuation in the wave amplitude. That was why we were scarcely able to watch any appreciable changes caused by the voltage wall.

Few interesting conclusions can be done more (we could try to change the shape of the barrier, its location, or add some more voltage walls), but all these possible modifications can be also made in 2D case, which is the main purpose of the present project.

CHAPTER 4. 2D SCHRÖDINGER EQUATION.

In the same way as we have already done in an unidimensional case, first of all we ought to try to develop both the numerical and the analytical methods for a furthermore comparison between them. Here, the consecution of both methods is explained step by step, as well as the results obtained during the process.

4.1. NUMERICAL METHOD

The Method of Lines (MoL) still remains as a chosen one for our purpose. Now, as it is a two-dimensional system, despite of having a quite same principle as in 1D, mathematically it is more complicated.

Let us consider a wave moving inside a rectangular of "a" length in X axis, and the length "b" in Y axis. The borders of such rectangular have an infinite voltage, so there is no possible wave there (denoted with a zero).

A two-dimensional Schrödinger equation for a single particle is written as:

$$i\hbar\frac{\partial\Psi(x,y,t)}{\partial t}=-\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi(x,y,t)}{\partial x^2}+\frac{\partial^2\Psi(x,y,t)}{\partial y^2}\right)+V(x,y)\cdot\Psi(x,y,t) \qquad (4.1)$$

Notice that, in a similar way as it was done in the unidimensional case, the voltage distribution does not depend on time.

The next step consists in leaving the equation in a dimensionless form. For such purpose, we start dividing all the equation both by the imaginary number i and the total energy of the particle, E.

$$\frac{\hbar}{E}\frac{\partial\Psi(x,y,t)}{\partial t}=\frac{i\hbar^2}{2mE}\left(\frac{\partial^2\Psi(x,y,t)}{\partial x^2}+\frac{\partial^2\Psi(x,y,t)}{\partial y^2}\right)-i\cdot V(x,y)\cdot\Psi(x,y,t) \qquad (4.2)$$

If we use the following dimensionless parameters (the sub index c means characteristic)

Dimensionless time $\mathrm{T}=\frac{t_c E}{\hbar}$

Dimensionless space parameters: $\bar{x}=\frac{x_c}{a}$ and $\bar{y}=\frac{y_c}{b}$

Dimensionless voltage (ratio between the voltage barrier and the energy available for the particle):

$$\bar{U}=\frac{V}{E}$$

We get the general expression below:

$$\frac{\partial\Psi(\bar{x},\bar{y},\mathrm{T})}{\partial\mathrm{T}}=\frac{i}{2}\frac{\hbar^2}{mEa^2}\frac{\partial^2\Psi(\bar{x},\bar{y},\mathrm{T})}{\partial\bar{x}^2}+\frac{i}{2}\frac{\hbar^2}{mEb^2}\frac{\partial^2\Psi(\bar{x},\bar{y},\mathrm{T})}{\partial\bar{y}^2}-i\cdot\bar{U}\cdot\Psi(\bar{x},\bar{y},\mathrm{T}) \qquad (4.3a)$$

If we denote a dimensionless constant $\chi=\frac{\hbar^2}{mEa^2}$, the equation takes the following form:

$$\frac{\partial\Psi(\bar{x},\bar{y},\mathrm{T})}{\partial\mathrm{T}}=\frac{i}{2}\chi\frac{\partial^2\Psi(\bar{x},\bar{y},\mathrm{T})}{\partial\bar{x}^2}+\frac{i}{2}\chi\left(\frac{a}{b}\right)^2\frac{\partial^2\Psi(\bar{x},\bar{y},\mathrm{T})}{\partial\bar{y}^2}\text{-i}\cdot\bar{\mathrm{U}}\cdot\Psi(\bar{x},\bar{y},\mathrm{T}) \tag{4.3b}$$

This is a general form of a dimensionless Schrödinger equation in 2D. Nevertheless, we are able to make a couple of assumptions that will simplify the problem during the comparison between the methods:

1) No change in the voltage is produced. This means that $\bar{\mathrm{U}}=0$
2) The grid is square (a=b), and χ is equal to zero

These assumptions transform the equation as follows:

$$\frac{\partial\Psi}{\partial\mathrm{T}}=\frac{i}{2}\left(\frac{\partial^2\Psi}{\partial\bar{x}^2}+\frac{\partial^2\Psi}{\partial\bar{y}^2}\right) \tag{4.4}$$

This form makes us easier the obtainment of the analytical solution, because the assumptions made above remain available for both methods.

The equation still remains a PDE. Therefore, we must go on with the discretization to transform it into an ODE.

It has been demonstrated yet (see 2.1) that the second derivative discretization has the next form, applied for both coordinated, and already dimensionless:

$$\frac{\partial^2\Psi}{\partial\bar{x}^2}=\frac{\Psi(\bar{x}-\Delta x,\bar{y},\mathrm{T})+\Psi(\bar{x}+\Delta x,\bar{y},\mathrm{T})-2\Psi(\bar{x},\bar{y},\mathrm{T})}{\Delta x^2}$$

$$\frac{\partial^2\Psi}{\partial\bar{y}^2}=\frac{\Psi(\bar{x},\bar{y}-\Delta y,\mathrm{T})+\Psi(\bar{x},\bar{y}+\Delta y,\mathrm{T})-2\Psi(\bar{x},\bar{y},\mathrm{T})}{\Delta y^2}$$

Where Δx and Δy represent the distance between the consecutive points in X axis and Y axis, respectively. It is observed that to manage the time evolution of the wave the surrounding points must be known, in both space dimensions.

At this point we face a major difficulty of the 2D case, in comparison with the unidimensional one: MATLAB is only able to solve the ODE functions for a vector, not for a matrix. The explanation of how to pass from one form to another, and vice versa is presented below:

Let us imagine a rectangular grid in two dimensions. In its X axis it is divided into (N_x-1) segments, while in Y axis into (N_y-1) segments. The distance between two consecutive points in the same axis remains constant, but it is not necessary that the distance between points in X axis (Δx) and in Y axis (Δy), were the same.

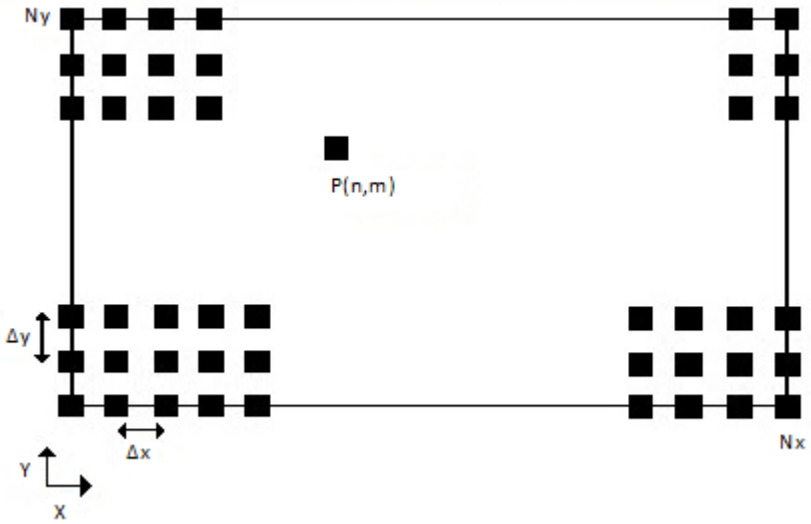


FIG 4.1. Schematic representation of the discretized two-dimensional space grid.

It is logical that the number of points both in its matrix and vector forms remains constant. So, if in a generic case we have a grid divided into N_x points in the X axis, and into N_y points in the Y axis, we should have a vector of $N_x \cdot N_y$ length, codificating the same points.

Now let us take the whole left vertical column, and assign its components as the first N_y points of the auxiliary vector. After that the second column is taken, and its points denoted as the elements of the vector going from (N_y+1) to 2N_y, and so on till completing the entire grid.

After that, one has to take care in taking the correct points of the vector. If in a matrix form an aleatory point P which occupies the position of the region (n,m), in a vector one it is designated as the (n-1)·N_y+m element. It is very important to make a clear difference between the constants N_x and N_y, which make reference to a total number of points in each axis, while n and m are the position coordinates of that point in the grid.

As it was said before, to be able to perform the time marching of the Schrödinger equation in 2D, we must know the value of all the surrounding points, both in X axis (the left and the right ones), and in Y axis (the upper and the lower ones). Here is a list which manages the transformation of an aleatory point and its surrounding ones from the matrix form to a vector one, and vice versa.

$$P_M(n,m)=P_v[(n-1)\cdot N_y+m]$$
$$P_M(n-1,m)=P_v[(n-2)\cdot N_y+m]$$
$$P_M(n+1,m)=P_v[n\cdot N_y+m]$$
$$P_M(n,m-1)=P_v[(n-1)\cdot N_y+m-1]$$
$$P_M(n,m+1)=P_v[(n-1)\cdot N_y+m+1]$$

Now that we are able to pass from one form to another, Dirichlet B.C. at the borders must be imposed, with the null value of the wave; in the same way an initial Gaussian wave packet is needed to start the iteration. We select its dispersive form, because it is easier to find an exact solution for the analytical method. In 2D its dispersive form is [3],[4]:

$$\Psi(x,y,0)=\frac{A\cdot\exp[(\bar{x}-\bar{x}_0)^2+(\bar{y}-\bar{y}_0)^2]}{\sigma^2} \qquad (4.5)$$

with:
A=constant that makes the probability of finding a particle in whole space equal to 1
$\ddot{x}_0$,$\dot{y}_0$=center of the Gaussian wave packet (its maximum value is here)
σ=width of the Gaussian wave packet
Once all the assumptions are made and all the conditions are imposed, MATLAB can solve the problem. The remaining thing is the transformation of a vector into a matrix to be able to visualize the results.

4.2. ANALYTICAL METHOD

As it has been told before, a Schrödinger equation is a PDE (Partial Differential Equation) itself, what means that is has dependence on time as well as on space. We start by assuming the same approximations we have already used in the MoL, providing us the equation (4.4):

$$\frac{\partial \Psi}{\partial T}=\frac{i}{2}\left(\frac{\partial^2 \Psi}{\partial \bar{x}^2}+\frac{\partial^2 \Psi}{\partial \bar{y}^2}\right)$$

Using the separation of variables method, we can split the initial equation into two equations, one relaying only on time and the other on space:

$$\Psi(\vec{r},t)=\psi(\vec{r})\cdot\varphi(t)$$

being φ(t) demonstrated in (1.10) as:

$$\varphi(t)=e^{-iEt/\hbar}$$

At the same time, the space equation also depends on two parameters, the X coordinate and the Y coordinate, so we have to continue using the separation of variables method:

$$\psi(\vec{r})=\psi(x,y)=X(x)\cdot Y(y)$$

It is important to take into account that in the analytical solution, the order of appearance along the X axis (denominated n) does not have to coincide with the order of appearance along the Y axis (m). Not to confuse with n and m referred to the number of discretized points in a numerical method.
After applying the B.C. as well as the normalization condition, we can find the eigenvalues and eigenvectors for 2D case (already dimensionless) [16]:

$$\psi_{nm}(\bar{x},\bar{y})=2\cdot\sin(n\cdot\pi\cdot\bar{x})\cdot\sin(m\cdot\pi\cdot\bar{y})$$

$$E_{nm}(\bar{x},\bar{y})=\frac{\pi^2}{2}(n^2+m^2)$$

Despite having the method of obtaining the eigenfunctions and eigenvectors, only few analytical solutions can be procured. We must use the superposition principle to allow us to get all the analytical solutions, as long as we can solve the Sturm-Liouville problem. We had simplified the problem by assuming no voltage barrier, the simplest problem, but still a reliable one.

$$\Psi(\bar{x},\bar{y},T)=\sum_{n=1}^{\infty}\sum_{m=1}^{\infty} c_{nm}\cdot\psi_{nm}(\bar{x},\bar{y})\cdot\varphi_{nm}(T)$$

$$\Psi(\bar{x},\bar{y},T)=\sum_{n=1}^{\infty}\sum_{m=1}^{\infty} c_{nm}\cdot 2\cdot\sin(n\cdot\pi\cdot\bar{x})\cdot\sin(m\cdot\pi\cdot\bar{y})\cdot\exp[-i\cdot\frac{\pi^2}{2}(n^2+m^2)\cdot T] \quad (4.6)$$

The only thing left is to get the matrix of constants (for each combination of n and m it has a specific value). This constant remains unalterable during the time. Hence, if we choose the same initial Gaussian wave packet as in the numerical method, we can make a double integration of it with "dblquad" function in MATLAB (available for the version of the year 2011; in the version 2013 it has been improved to the "integral2" function, so we can get a matrix of size (n x m) for the constants.

4.3. COMPARISSON BETWEEN THE METHODS

Once both numerical and analytical methods are developed, it is time to overlap them together to observe the results, in order to confirm the validity of the numerical script. As the wave is a complex number, we should better compare the probability results (multiplying the wave by its conjugate). It is not possible to take a clear account of the overlapped results with the "mesh" functions; therefore, we must improve another ways to prove the validity of the numerical method.

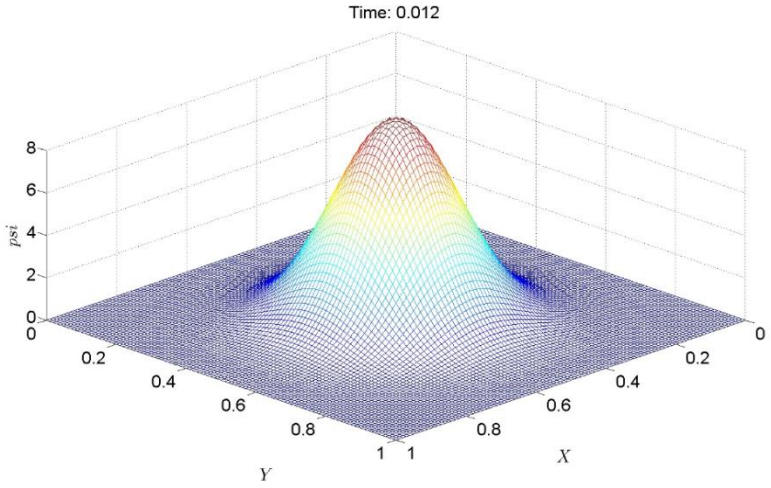


FIG 4.2. Mesh grid for a two-dimensional wave probability

The easiest and the simplest process, but also a most rudimentary one, consists in taking some aleatory points in the space grid for certain intervals of time, and comparing the results given by both methods one by one. To avoid coincidences that might give us mistaken results, the amount of such points has to be quite numerous, as well as they also have to been taken in many different times. The following chart provides us some of these points. As we can see, the results given by both methods are quite similar.

T	χ	ϒ	Analythical	Numerical
0.005	0.45	0.45	19.4094	19.3813
0.005	0.60	0.50	11.7742	11.7598
0.005	0.40	0.60	4.3310	4.3115
0.005	0.33	0.65	0.1873	0.1853
0.008	0.53	0.48	16.7117	16.8428
0.008	0.41	0.59	7.2354	7.2477
0.008	0.64	0.64	1.9874	1.9815
0.008	0.57	0.39	6.9180	6.9246
0.010	0.53	0.47	11.9114	12.0528
0.010	0.38	0.52	7.0808	7.1290
0.010	0.46	0.49	11.9586	12.0120
0.010	0.50	0.55	11.5832	11.6391
0.012	0.50	0.50	9.4678	9.5322
0.012	0.52	0.38	6.1108	6.1496
0.012	0.68	0.61	2.5384	2.5485
0.012	0.40	0.53	6.8584	6.8552

CHART 4.1. Contains the rudimental comparison by taking an aleatory point and aleatory time and compare the numerical solution with the analytical one.

A more sophisticated method of comparison is based on the use of the “contour” function. It consists in representing the probability of the wave in a two-dimensional plot. It can be said that it make some kind of “topographic map” of the probability. In such way we can overlap the results of both methods for the same time and make a contour plot for several values of time.

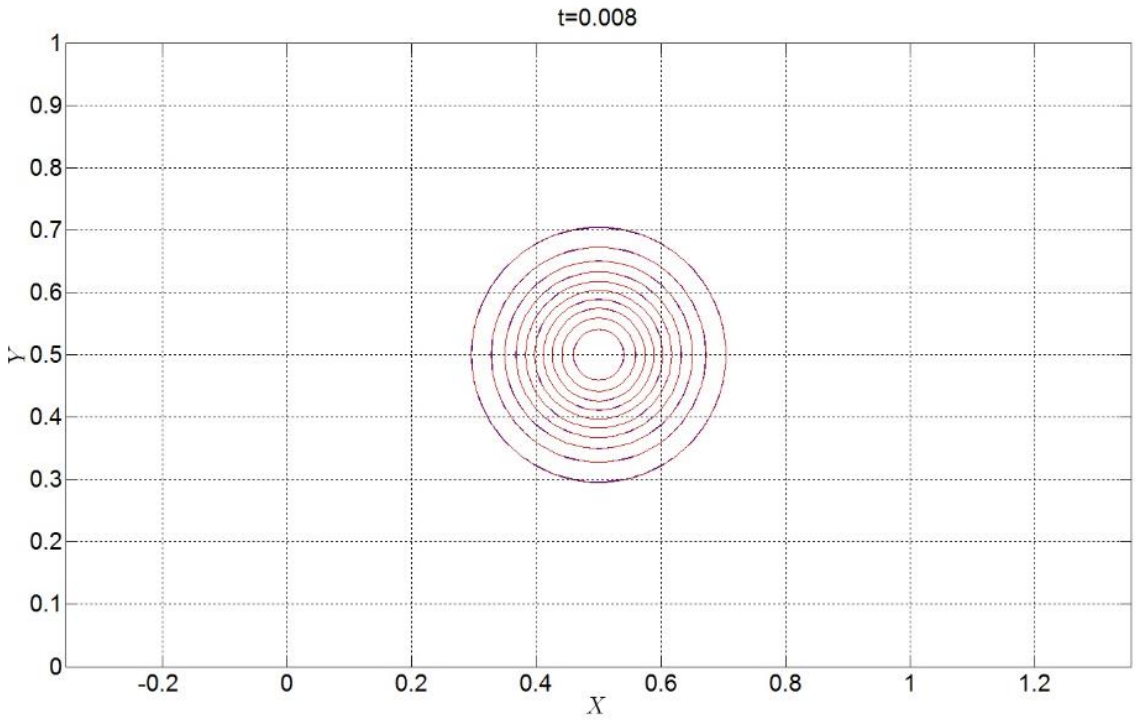


FIG 4.3. Contour for both methods at T=0.008. In the same way as in a comparison plot for a unidimensional case, the numerical solution is represented by red and the analytical by blue. The coincidence is very high.

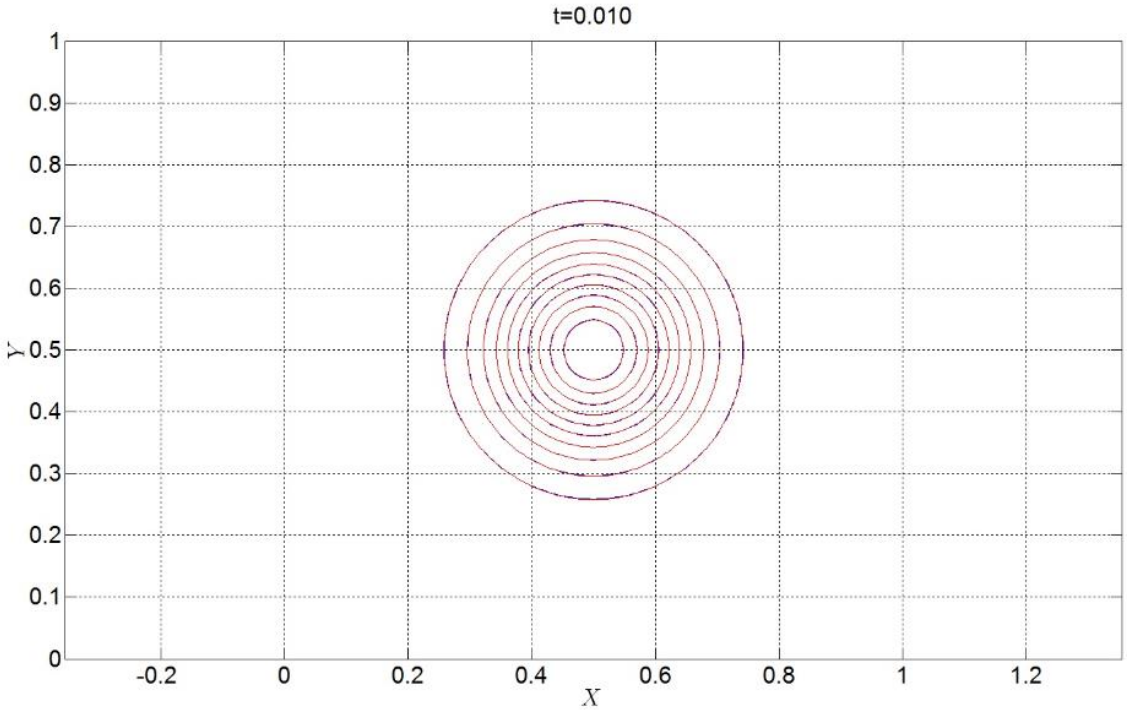


FIG 4.4. T=0.01. The initial wave packet continues splitting without any anomaly.

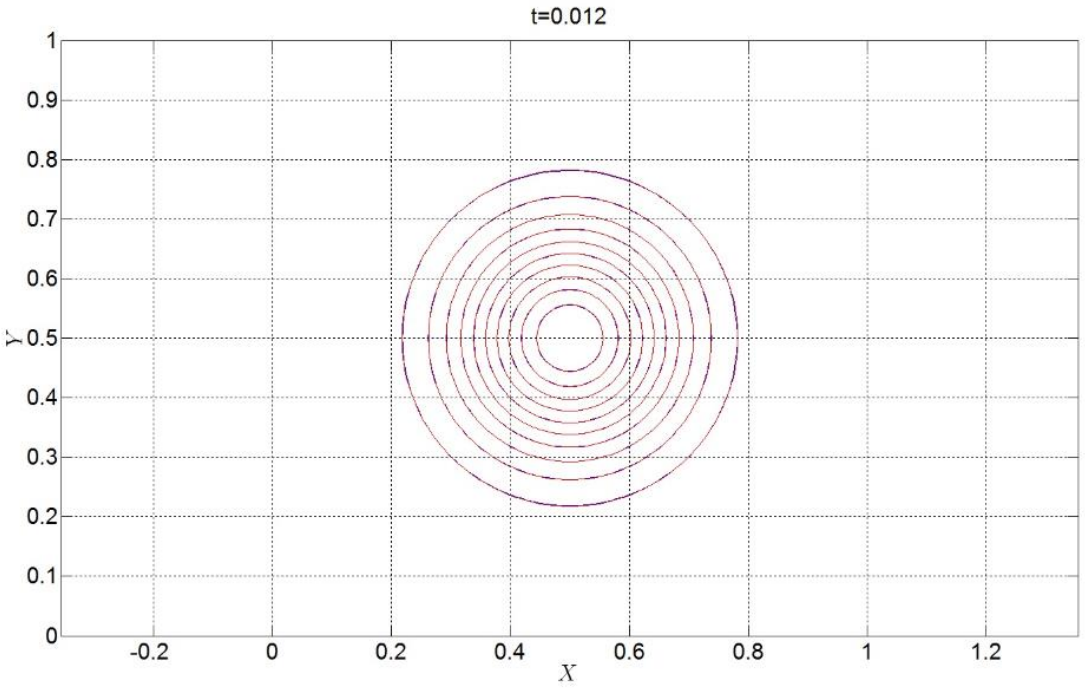


FIG 4.5. T=0.012

Now, once we have proved the truthfulness of the chosen numerical method (MoL), it is time to move on by imposing some voltage barriers. There are three cases on which we have centered our attention: an aleatory voltage barrier; a barrier with a slit in the direction of the movement of the wave; the previous case but with two slits instead of one.

4.4. AN ARBITRARY VOLTAGE BARRIER

For this simulation we have continued with the grid we have developed during the introduction to the MoL; that means there is a square dimensionless grid with a=b, and an initial Gaussian wave packet located in the center of such grid at $\bar{x}$=$\bar{y}$=0.5, being the previous parameters dimensionless lengths in X and Y axis respectively. The wave itself is a dispersive one, spreading equally in all directions.

To impose the voltage barrier we must choose its space distribution as well as its height (it is better said the quotient between the height of the barrier and the total energy of the particle, due to the fact we have made the whole equation dimensionless). The voltage ratio does not have to be too low so that the wave could not overstep it freely (there must be some attenuation in the wave, with some part of it passing through the voltage "wall", meanwhile the rest of the wave rebounds backwards), but it also should not be too high so that the wave was not able to pass it. Therefore, we must seek for such range of values that let us observe the results of the tunneling phenomenon in 2D and make subsequent conclusions. The chosen value of the barrier is $\bar{U}$=250. Although it might be seen as a very large voltage, as we perform the time marching we can observe that an important part of the initial wave oversteps the barrier. One possible reason of this behavior is the little width of voltage region (see TRANSMISSION QUOTIENT).

Regarding to the voltage distribution, we have chosen a cross-shape one. We must take care in not placing the barrier too close to the initial Gaussian wave packet, because it may bring some problems as we start the numerical simulation.

Another important point referred to the numerical strategy is the convenience of smoothing the voltage barrier, as MATLAB may have some problems if there were an abrupt change in the voltage value. To manage to avoid such complication, we should write the voltage as a hyperbolic function for every axis. For example, if we want some barrier stretching along the generic dimensionless coordinates $\bar{x}_1$ and $\bar{x}_2$ in the X axis (independently of the Y axis), it takes the next form:

$$\bar{U}(\bar{x})=\bar{U}\cdot 0.5\cdot\{\tanh[\beta\cdot(\bar{x}-\bar{x}_1)]-\tanh[\beta\cdot(\bar{x}-\bar{x}_2)]\} \tag{4.7}$$

Where $\bar{x}$ denotes the position of all the points of the X axis. If the value β is big enough, its height is most likely seen as the one with the square form, with constant voltage in the dominion delimitated by $\bar{x}_1$ and. This is in boundary points, named $\bar{x}_1$ and $\bar{x}_2$, with the barrier the middle of the normal height, where the smoothness occurs, avoiding any change that might be damaging for the simulation. The same thing must be done for the Y axis, and the final voltage obtained by this method is the result of the multiplication of $\bar{U}(\bar{x})\cdot\bar{U}(\bar{y})$

Like it has been explained before, to be able to perform the time marching with ODE45 function, we have to pass the voltage matrix distribution to a vector form, without any further complication we were able to observe.

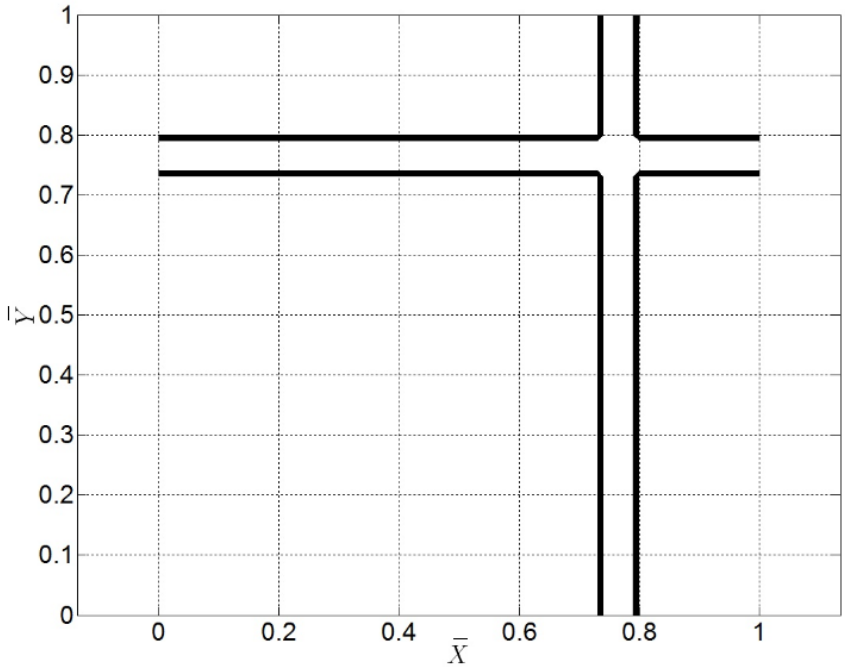


FIG 4.6. The voltage barrier seen from above.

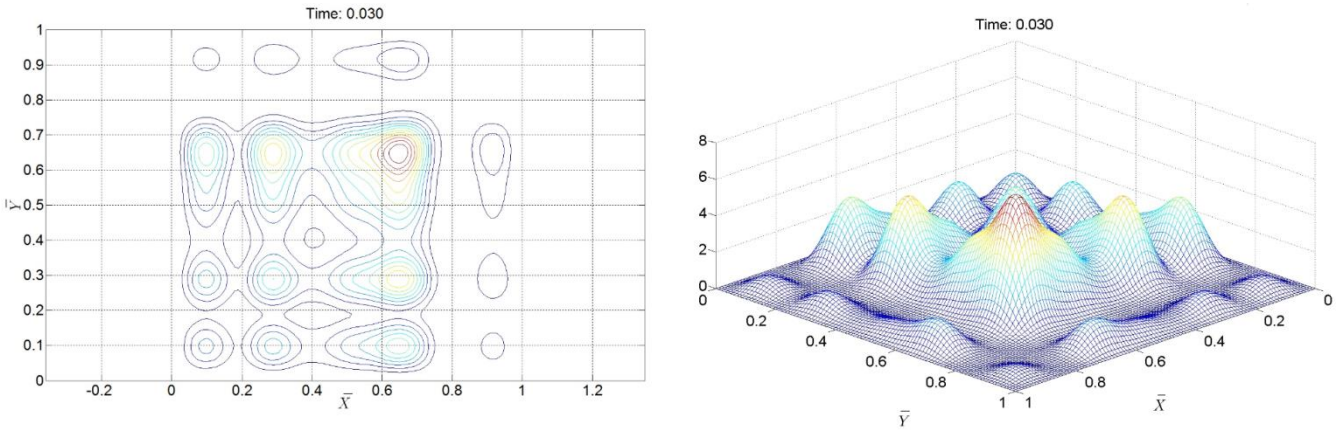


FIG 4.7. The shape of the wave at T=0.03, represented by a "contour" and "mesh" plots. Notice that for the "mesh" one we have turned it over to observe the phenomenon of the quantum tunneling from a better angle, also done in all the following simulations. No rebound from the grid boundaries has yet occurred.

Finally, it is quite recommendable to check whether if the probability of finding a particle in all space grid remains constant and close to the unity (or 100 %) during the simulation.

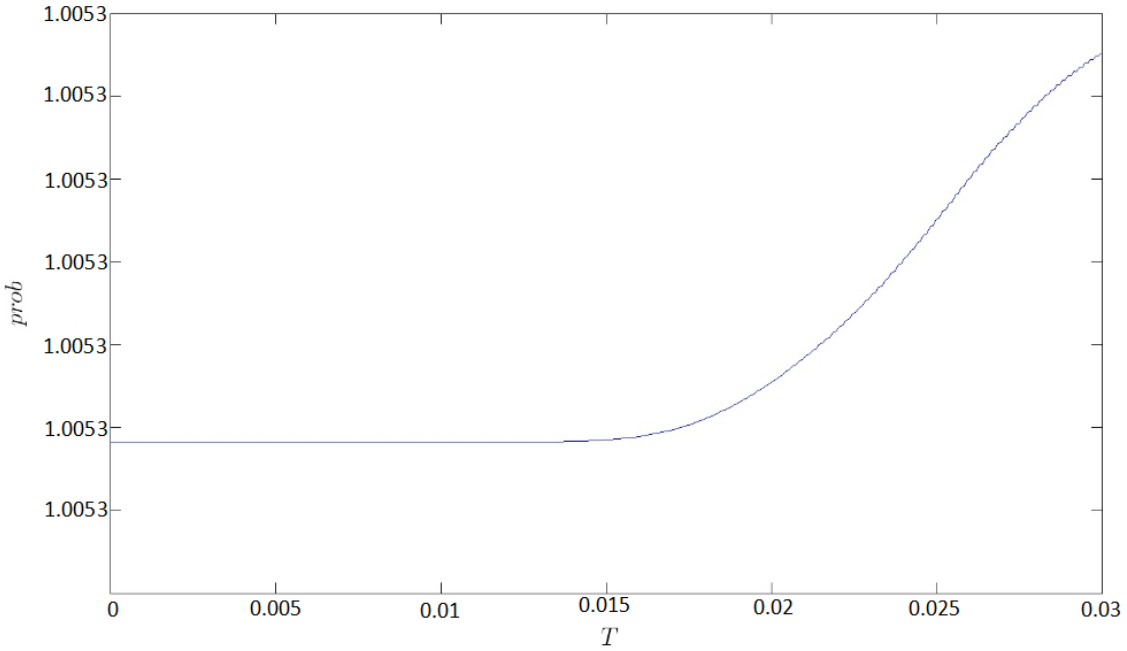


FIG 4.8. Probability vs time

As it can be observed, the probability has hardly changed, maintaining its values around 1.0063, not even changing the last number, what means an error of less than 0.01%. The decimals are caused by a non-exact initial normalization.

4.5. ONE SLIT BARRIER

Now we will center our attention and efforts on a special kind of barrier. Imagine a straight barrier which stretches over completely from one side to another, being parallel to one of the axis; let us assign it as the Y axis. That barrier has a voltage ratio so high that the overstepping

of the wave over it practically does not exist. Despite of that, there is a small region of the barrier where the value of the voltage drops to zero; this is, the wall is considered almost solid, except a small gap where the voltage is non-existent. We use the hyperbolic functions to smooth in some way the abrupt change in the value of Ū, which is Ū=20000.

On the other hand, there is a nondispersive Gaussian wave packet moving over the X axis, along the line perpendicular to the barrier and which passes through the slit. To obtain a nondispersive form of the wave, we consider that the phase velocity shall maintain constant. It can be obtained multiplying the wave wholly by the parameter referred to the X axis (as it is the direction of the movement of the wave) [8][9]:

$$\exp(i\cdot k\cdot \bar{x}) \tag{4.8}$$

being:

i= imaginary number

k= de Broglie wavenumber

$\bar{x}$= dimensionless parameter along X axis

The wavenumber is a property of the wave vector, describing the frequency of the vibration of the wave for certain distance. The wave vector is composed basically by a direction, in our case the X axis, meanwhile its magnitude is given by the wavenumber. It has some relation with the energy of the particle, because it is also the inverse of the wavelength (commonly referred by the letter λ) [18].

$$k=1/\lambda$$

or, due to its sinusoidal form, it can be written as:

$$k=2\pi/\lambda$$

It is also well known that the total energy of the particle depends inversely on the wavelength. This relation between the energy of the particle and the wavelength (and therefore with the wavenumber) is expressed by the de Broglie's equation [19]:

$$E=\frac{\hbar}{\lambda}=\hbar\cdot k \tag{4.9}$$

with:

E= total energy available for the particle (in J or electronvolts)

ħ= Planck constant; $6.626\cdot 10^{-34}$ J·s

λ= wavelength (expressed with space unities)

k= wavenumber (inverse of the wavelength)

On the other hand, the total energy can also be described as:

$$E=m\cdot v_0 \tag{4.10}$$

being:
m= particle mass
v_0= particle linear velocity

This means that the wavenumber has a direct influence both on the total energy of the particle (remember that we have made the equation dimensionless, so the height of the barrier is related with the energy of the wave by the number Ū), and on the particle speed with:

$$v_0=\frac{\hbar \cdot k}{m} \tag{4.11}$$

Returning to our simulation with a unique slit in the voltage wall, we are going to modify the dimensions of the grid to regard better the movement of the wave. Therefore, we make the coordinate X (along the movement of the wave) four times as long as the coordinate Y. In that way we can observe better all the effects produced by the movement of the wave packet and specially its behavior in the region next to the slit. This change in the dimensions can easily be done by modifying the parameters "a" and "b", which are responsible of the length in X axis and Y axis, respectively (see the equation 4.3b). So, imposing a value of four for $\bar{x}$ without changing $\bar{y}$ we get our purposes, as it is done in our simulation. According to this modification, we can place our barrier and the initial wave wherever it is more convenient for a good visualization of the results. The position of the Gaussian wave packet remains centered in $\bar{x}$=$\bar{y}$=0.5; the barrier is located in the region 0.95<$\bar{x}$<1.05, stretching over the entire Y axis except a small region without any voltage in the middle, so the slit lays in the trajectory of the movement of the particle.

The chosen wave has a diameter a bit larger than the width of the slit, making easier that once it crashes against the voltage wall, some of it rebounds in the other direction, while the other part passes through the gap and splits over in all the directions. The diameter is regulated by the value of sigma (σ), imposed by us as σ=0.1. If the wave is too big in comparison with the slit, very little amount of it passes through; and if it is too small, the packet keeps on travelling without any influence of the barrier.

It is interesting to observe how the wave gets stuck for a moment in the slit, concentrating a huge amount of the wave in it (as it is logical, for a smaller opening it has more difficulties to pass through, and more wave probability is located there). Moreover, we have observed it also has more or less difficulties depending on the wavenumber value. With small values, and therefore with less speed and less energy, the wave barely passes through the slit. The optimal values of the wavenumber remain around 100-200. After passing the slit, the wave splits forward in all directions (remember that initially it was a non-dispersive wave moving along a determined line in the X axis).

4.6. ONE SLIT SIMULATION RESULTS

For the different analyzed cases, we have modified some parameters such as the wavenumber (k) or the slit width, remaining others, such as σ and the ratio of height Ū, constant for each simulation. Both mesh and contour plots for different times are given.

K=60 and the slit located between 0.49<$\bar{y}$<0.51

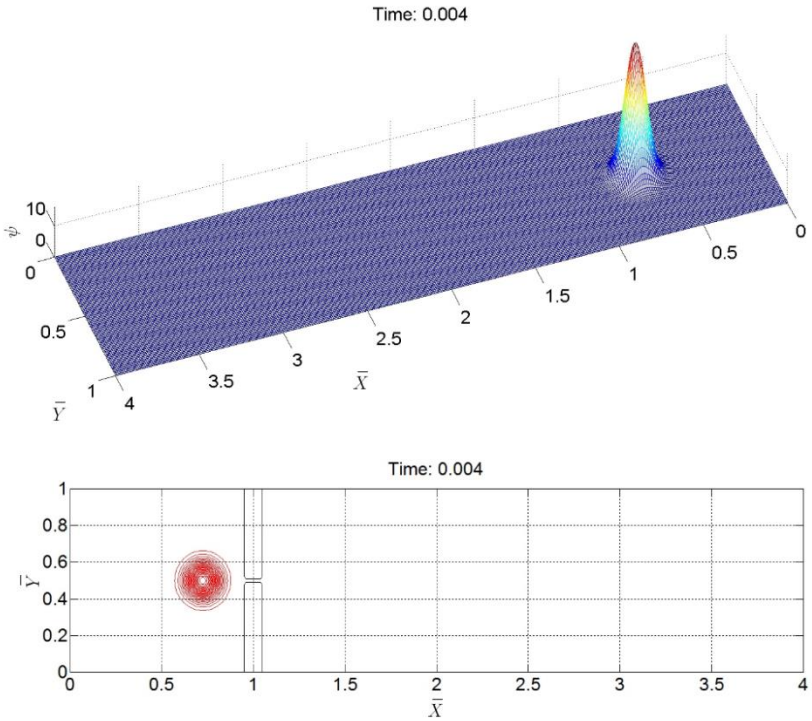


FIG 4.9. T=0.004. As it will be noticed comparing with the future simulations, the wave is moving much slower than with higher values of the wavenumber

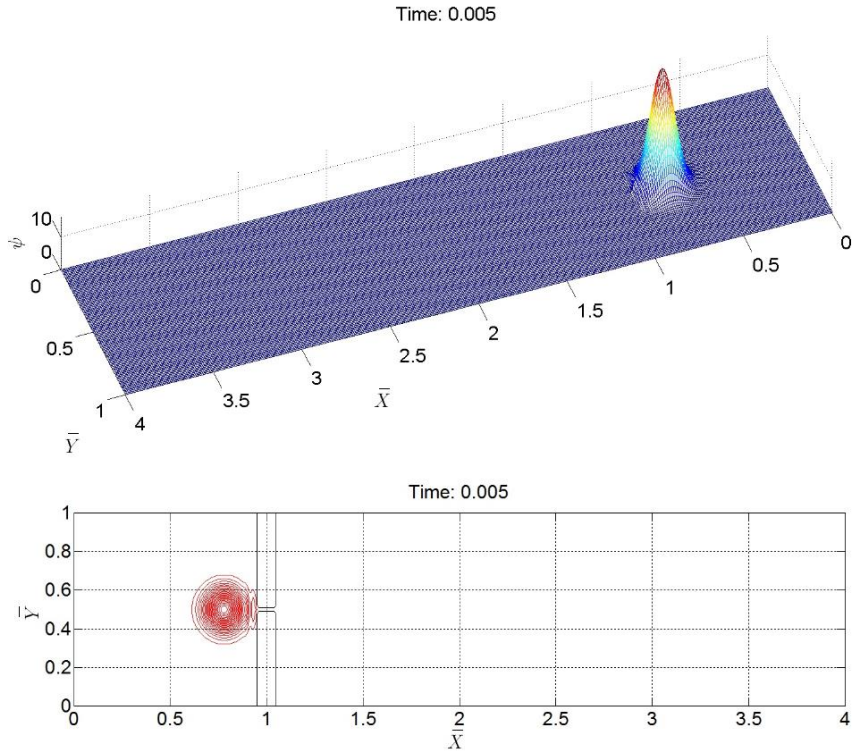


FIG 4.10. T=0.005. The wave impacts the barrier, best observed in the contour plot

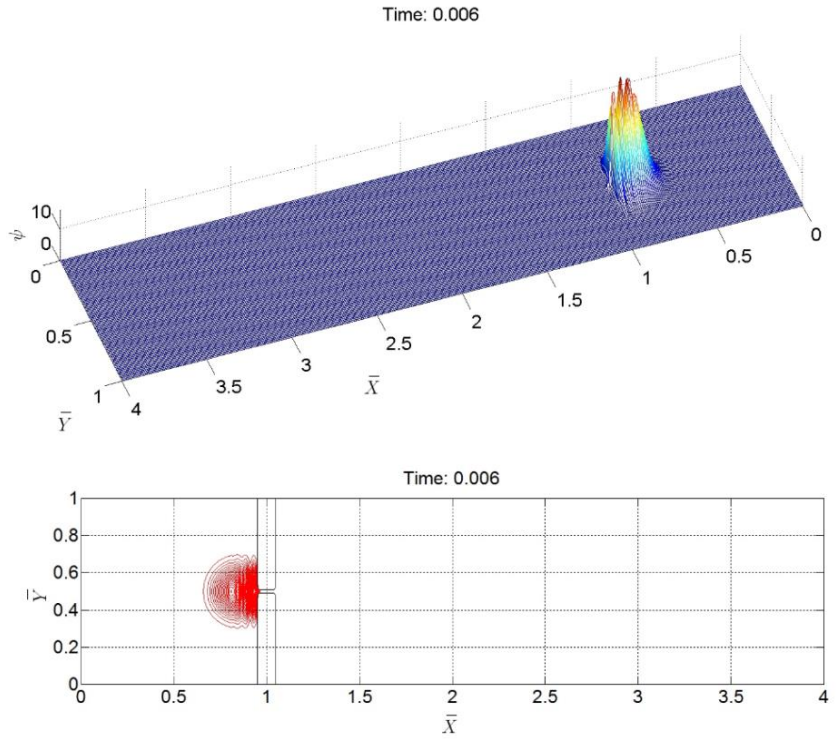


FIG 4.11. T=0.006. It still cannot go through in the slit

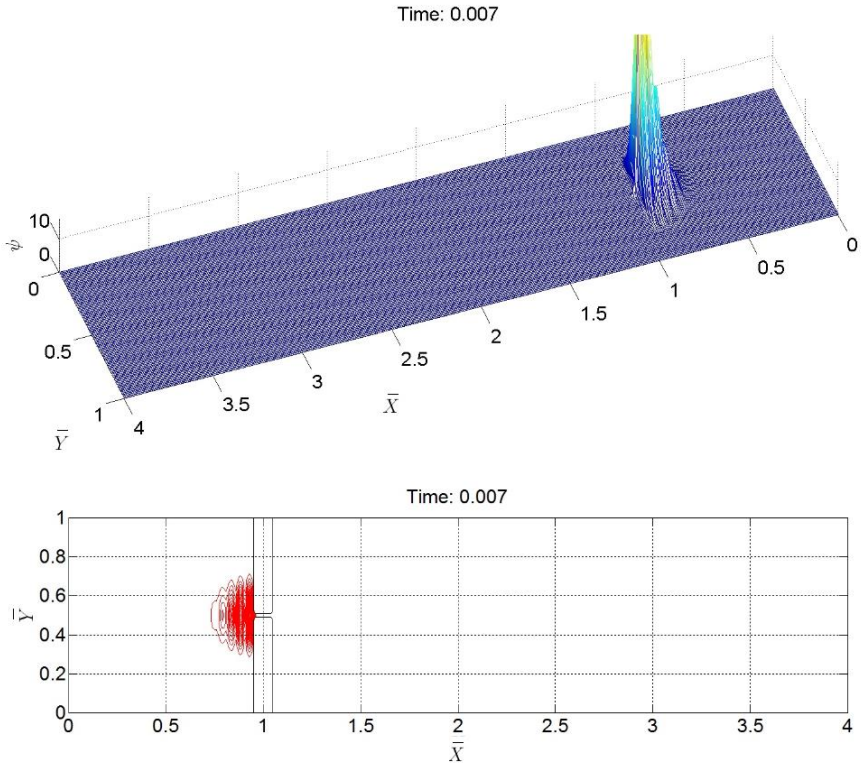


FIG 4.12. T=0.007. The wave is too “huge” to notice the barrier and pass through it, so it is being compressed at the entrance.

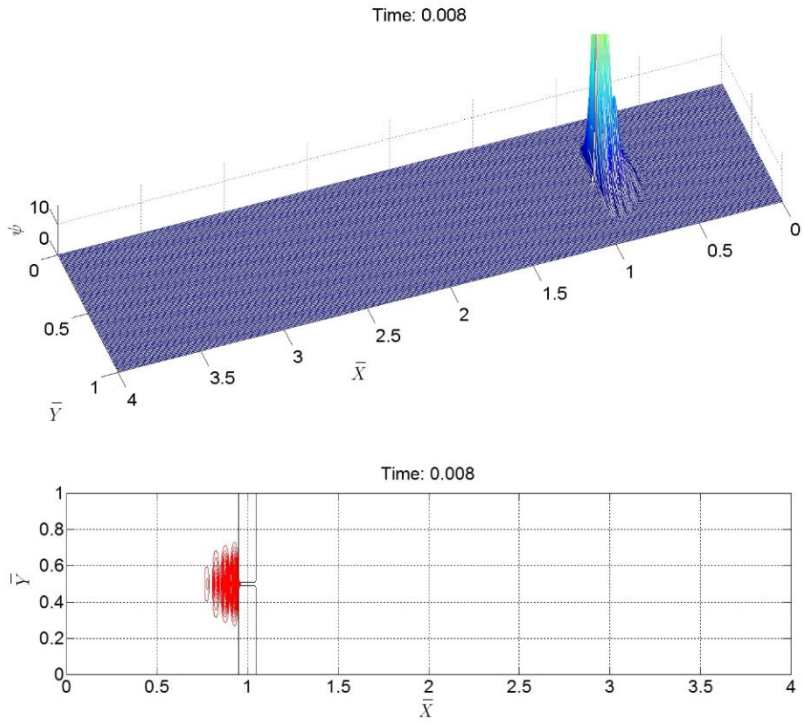


FIG 4.13. T=0.008. The wave is still next to the barrier, decreasing the space it occupies, and therefore increasing the amplitude to conserve the probability

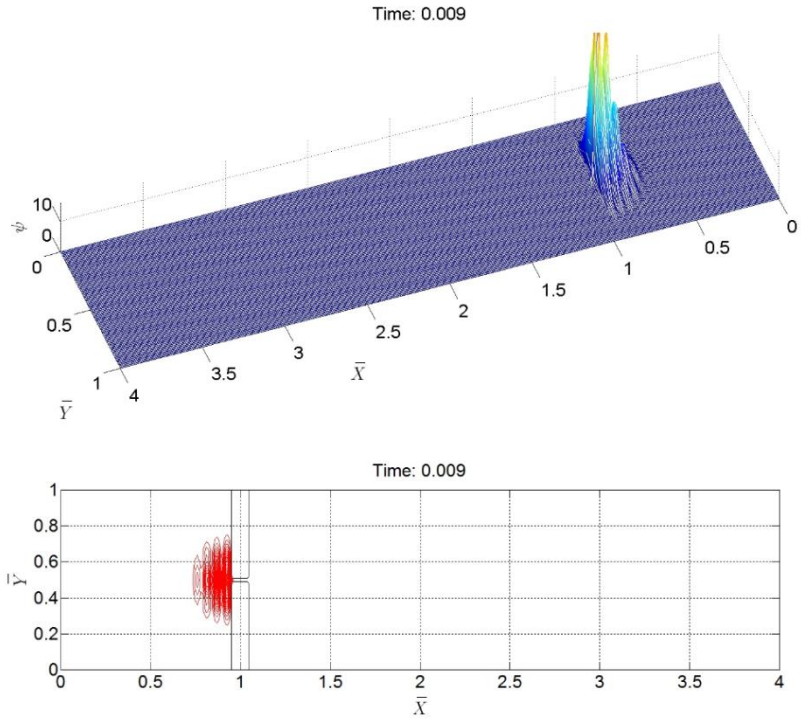


FIG 4.14. T=0.009

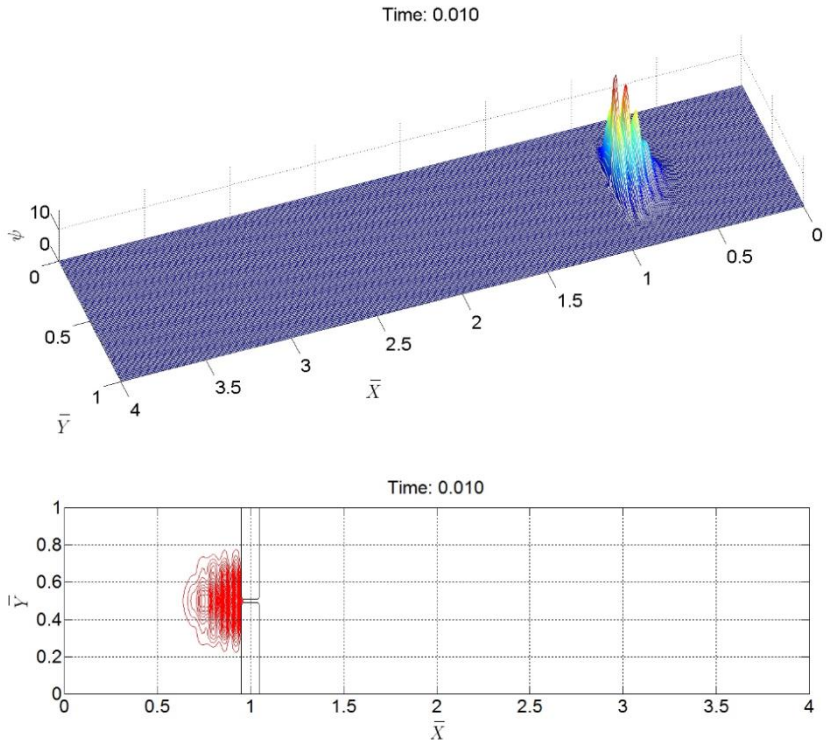


FIG 4.15. T=0.01. The barrier begins to withdraw without having penetrated the slit.

Finally, the normalized probability is included here

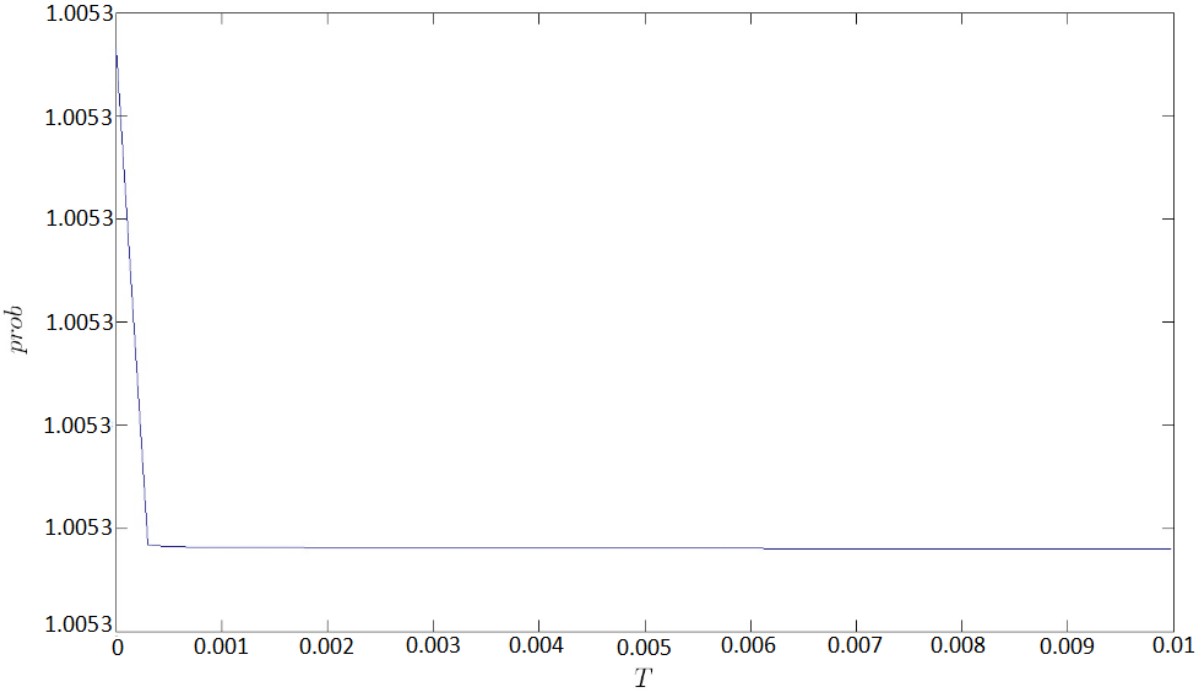


FIG 4.16. The variation is almost insignificant.

K=200 and the slit located between 0.49<Y<0.51

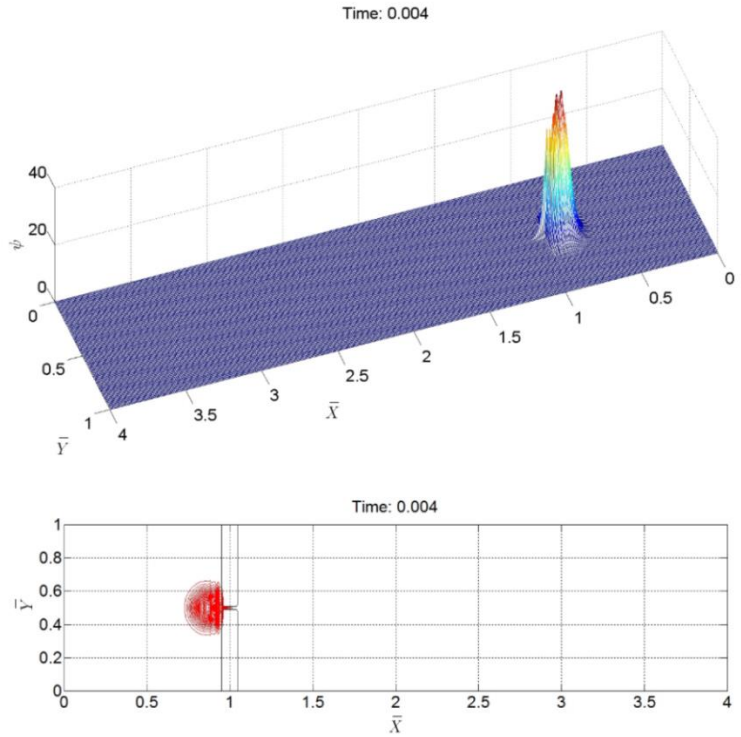


FIG 4.17. T=0.004. The wave crashes into the barrier. It has arrived much faster due to a larger amount of energy, and hence more speed it has.

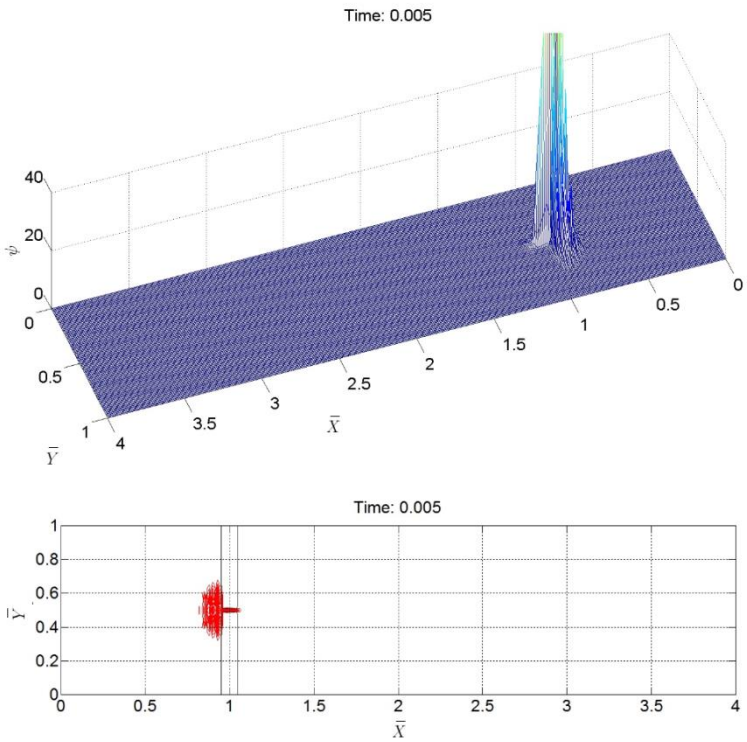


FIG 4.18. T=0.005. The wave starts to pass through the barrier; meanwhile the part moving behind compresses the forward part, increasing its height and pushing it to the gap.

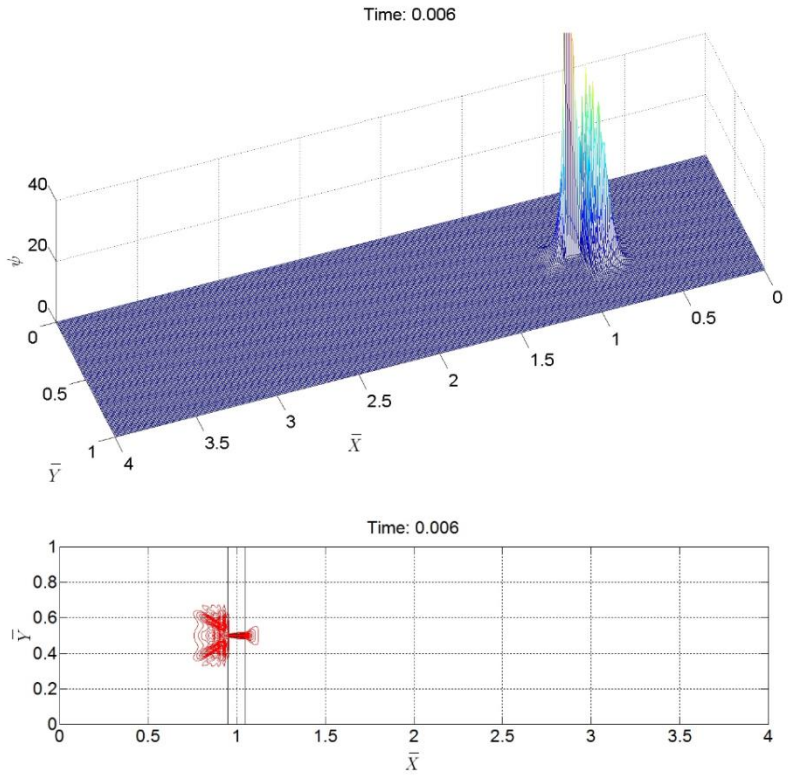


FIG 4.19. T=0.006. One part of the wave passes through the slit, some rebounds at the barrier and starts moving backwards (decreasing its probability modulus), and the other is still confined in the slit.

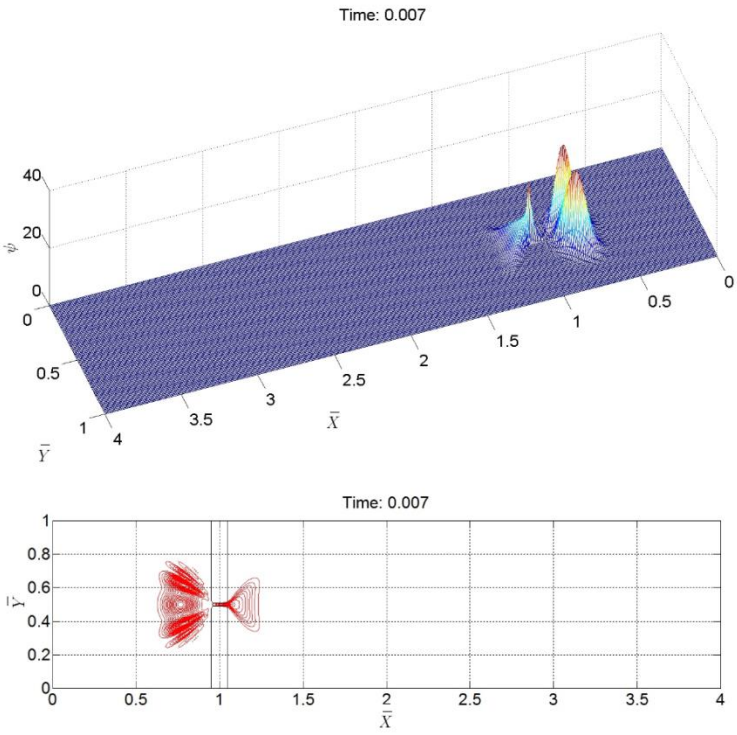


FIG 4.20. T=0.007. The wave which has passed through the wall, as well the one which has been returned back, start splitting in all directions, losing their non-dispersive nature.

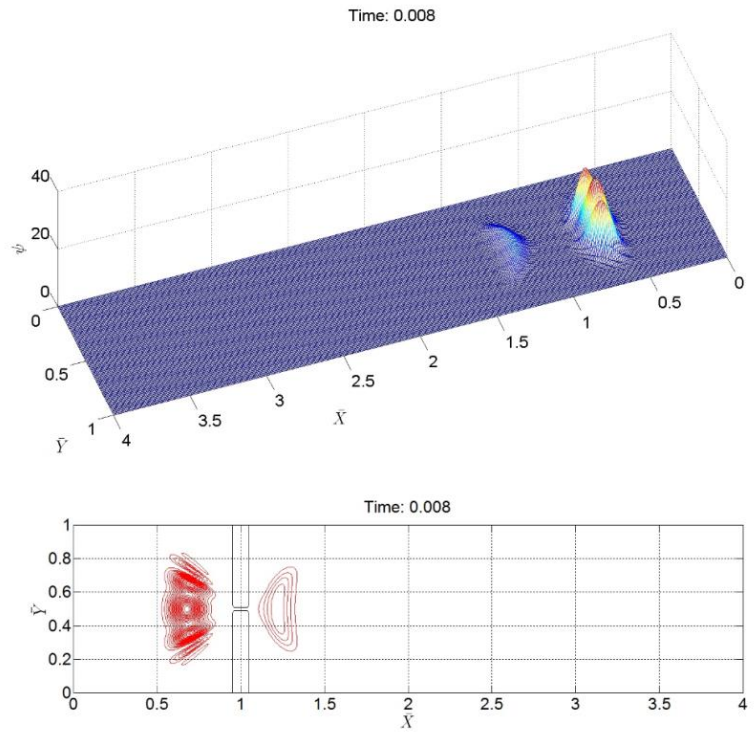


FIG 4.21. T=0.008

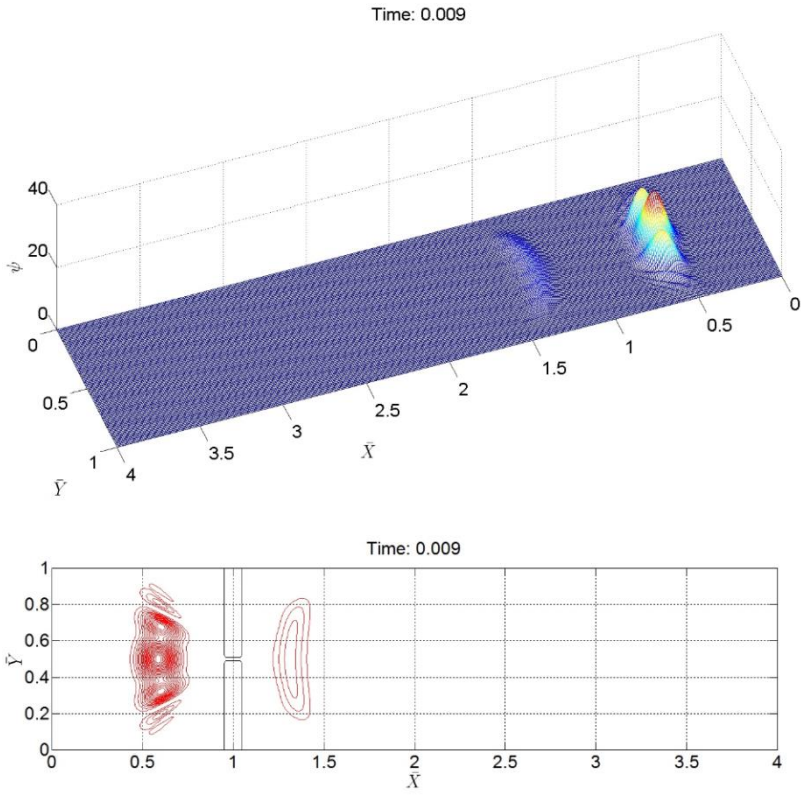


FIG 4.22. T=0.009

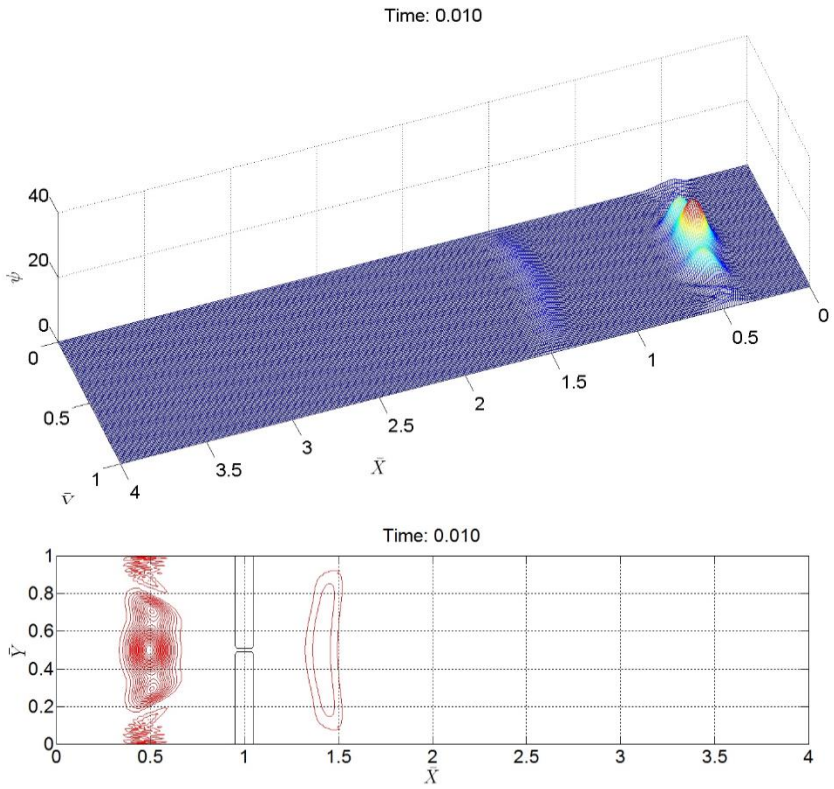


FIG 4.23. T=0.01. The wave starts to crash against the sides, perturbing the results. Furthermore, as we have already observed its pass through the slit, the subsequent simulation has no practical interest.

After all the time marching, it would be recommendable to prove whether if the probability of finding a particle in all space grid still remains and close to one (or in other words 100%).

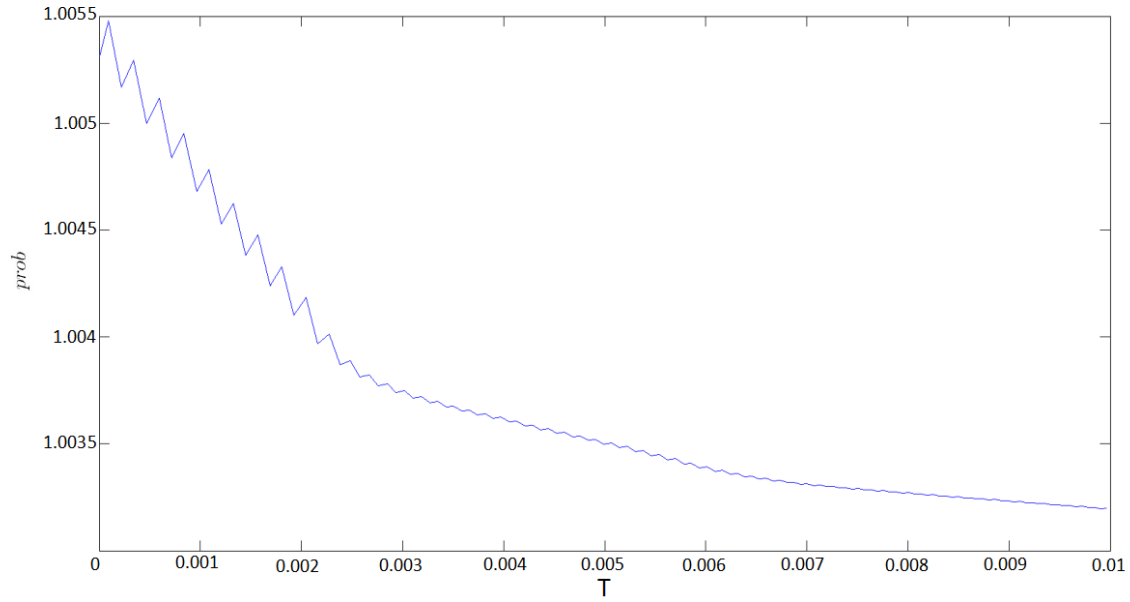


FIG. 4.24. Here a part of the graphic has been extended to watch better the results. The variation in the probability is of about 0.002, or what is the same, of 0.2% relative, so in this case we can confirm the probability results to be as the valid ones.

K=200 and the slit located between 0.48<ϒ<0.52

We have increased the width of the slit to regard the behavior of the wave once the quotient between the diameter of the Gaussian wave packet and the measurement of the gap is reduced. There are no visible changes in respect of the previous case till the moment the wave goes through the opening around Ƭ=0.008. Unlike the simulation before, there is a certain part of the probability "confined" in the gap, moving neither forward nor backward. As the simulation goes on, it slowly dissolves, but a certain part of it still remains trapped there.
This effect is best observed in the contour plot.

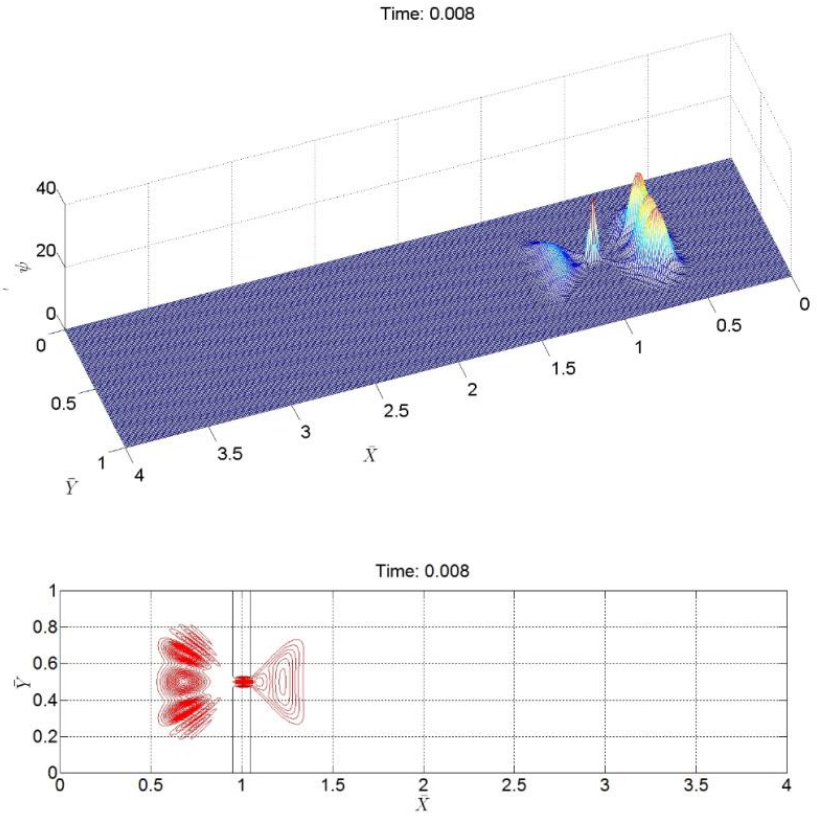


FIG 4.25. Ƭ=0.008. The wave after passing through the barrier

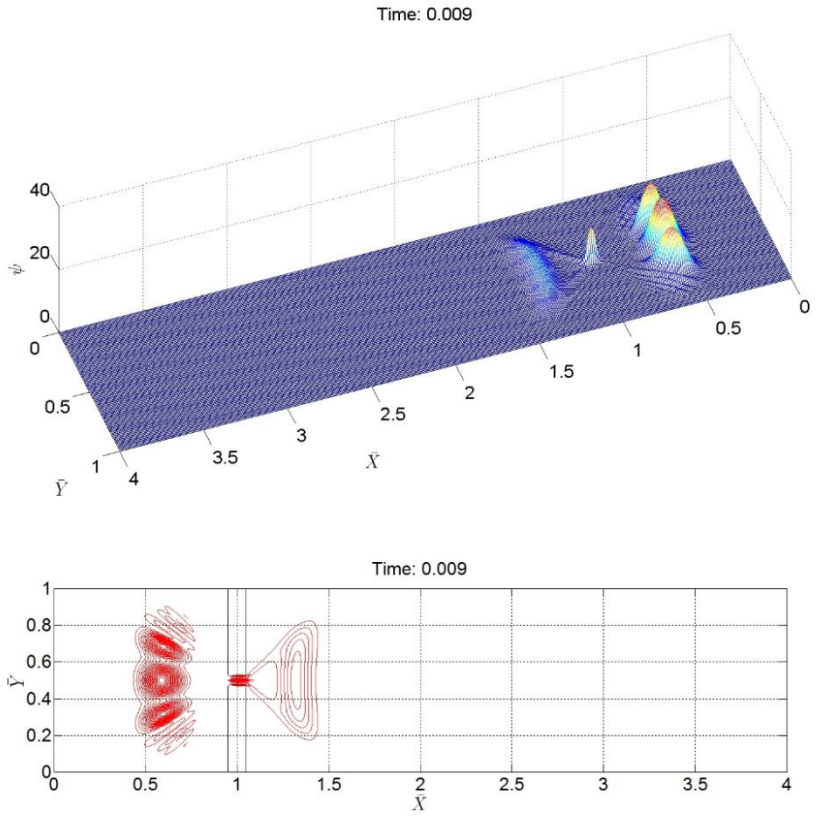


FIG 4.26. T=0.009.

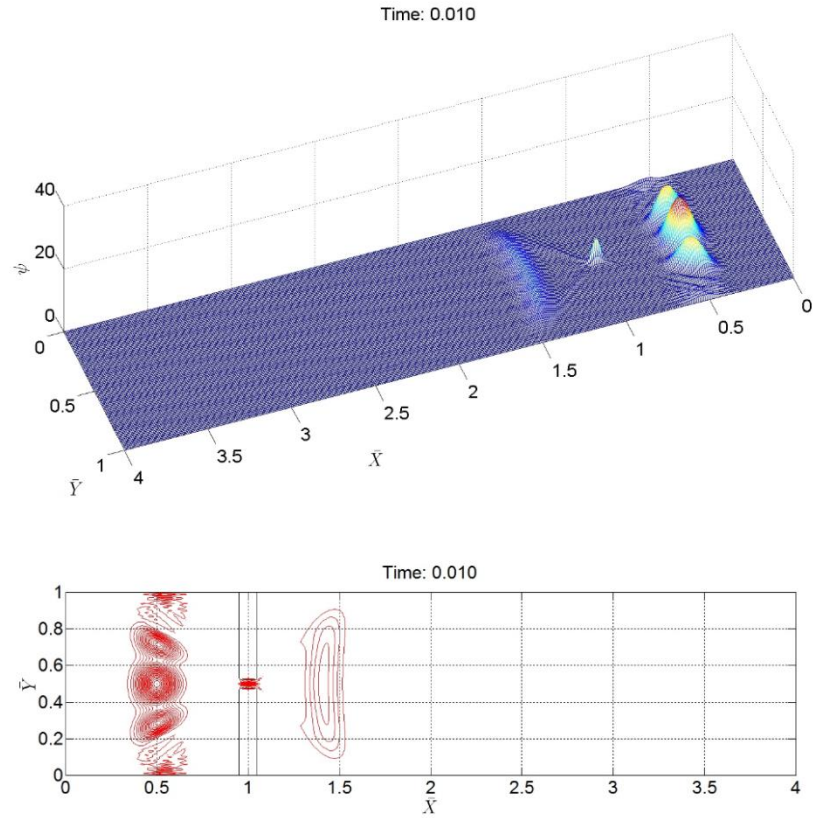


FIG 4.27. T=001. We do not know exactly why this phenomenon occurs. Perhaps a bigger amount of the wave which passes through the slit creates some kind of “probability jam”, but it is not yet clear.

4.7. A NOTE APART: WAVENUMBER AND ITS VALUE

In the cases we have already simulated for one slit barrier, the chosen value of the wavenumber has been 200. In double slit barrier the wavenumber is 100, making the movement more slow so we could observe all the phenomenon related to the case with more precision and detailing. Nevertheless, once we try to modify it, curious things begin to happen. If its wavenumber is too low (around 10-20), the wave does not have enough energy to go through the grid and the wave rebounds wholly as if the gap doesn´t exist. Increasing its value, it begins to pass easier through the slit, thing which might seem reasonable as the wavenumber has an influence on the energy of the particle, and therefore on its speed. That is why we have selected wavenumbers with a worth of few hundreds. But as we continue increasing the wavenumber, for a certain value the initial wave packet suddenly starts to move in the opposite direction! To try to explain this numerical phenomenon, we have tried to apply some possible theories (although none of them has been totally proved or denied):

1) The velocity of the wave packet is relativistic, that is, close to the light speed. The speed has the following dependence with its mass, the Planck constant and the wavenumber:

$$v_0=\frac{\hbar\cdot k}{m}$$

As the Planck constant maintains always the same value ($6.62\cdot10^{-34}$J·s), it shows us that a particle with less mass has a faster speed, as long as its wavenumber remains constant. Theoretically, one of the smallest particles which obey the Schrödinger principle is an electron, with a mass of $9.1\cdot10^{-31}$kg. Using the wavenumber of 1000, and replacing the parameters with their numerical values (it is better to use the order of magnitude), we have:

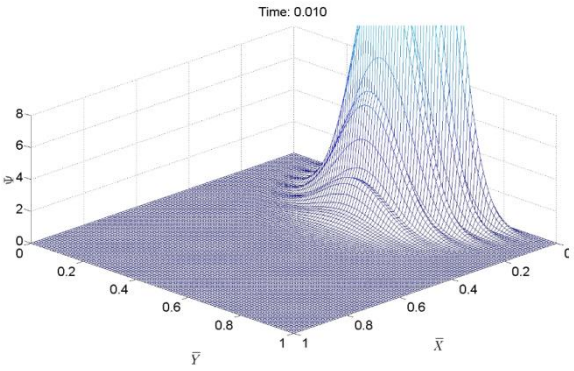
$$v_0=\frac{10^{-34}\cdot10^{3}}{10^{-31}}=1$$

This means that with a given wavenumber, a particle still moves only few meters per second, what seems to reject this theory. Furthermore, the light speed has no effect on the numerical simulation (it has a physical effect, but this is quite irrelevant for MATLAB). Therefore, it can be concluded that this first suggestion is very improbable, but we have not totally refused it.

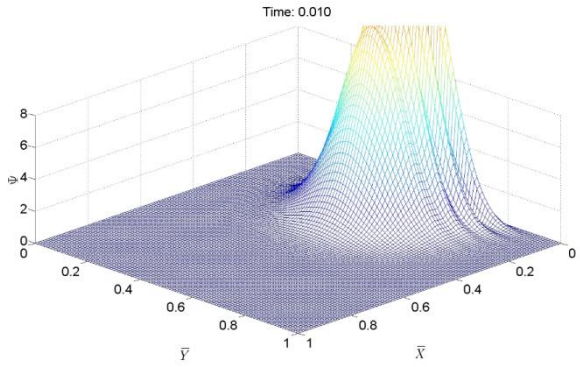
2) A wave vector goes gradually changing the direction. Any wave has a wave vector associated to it [20]; by definition it is a vector which helps us to describe a wave, whose magnitude is a wavenumber [18], and being its direction the direction of wave propagation.

There are some cases, probably the one studied is one of them, in which the wave vector may not point exactly in the direction of the wave movement. The wave propagation is the direction which is followed by the Gaussian wave packet (in other words it is the direction of the group velocity), meanwhile the wave vector is pointing in the direction of phase velocity (definition: the velocity at which the phase of any frequency which composes a wave travels). Therefore, the direction of the movement of the particle is always constant along the X axis (because we have chosen so), meaning that the group velocity is the same, the wavenumber may have some influence on the direction of the phase velocity, and with it its projection over the X axis suffers changes, being responsible that the modulus over the X axis and the direction

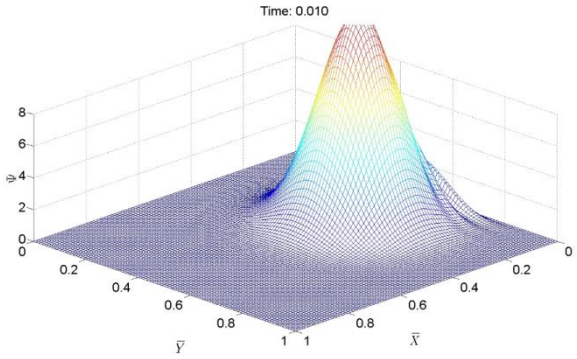
of the propagation of the packet go varying. This argument is reinforced as we gradually change the value of the wavenumber and observe the results. In order to observe easier the results, we simulate a movement of a Gaussian wave packet, initially located at $\bar{x}$=$\bar{y}$=0.5 (the grid is has both dimensionless space parameters equal to the unity), and observe the time marching till T=0.01, changing only the wavenumber k.



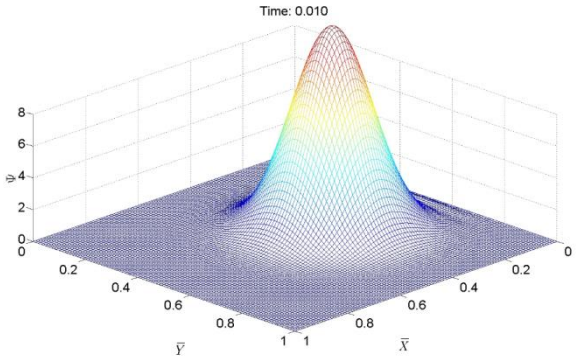
k=270



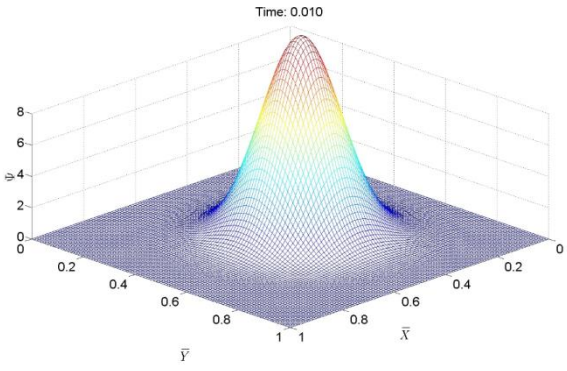
k=280



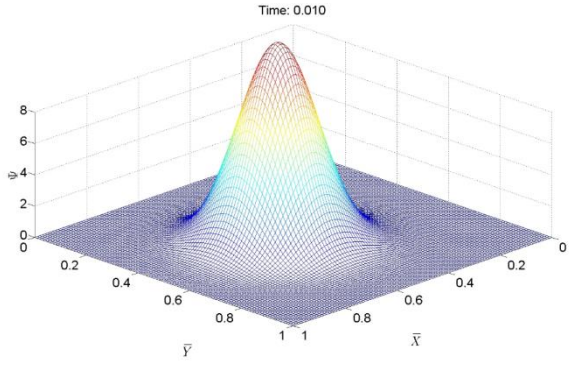
k=290



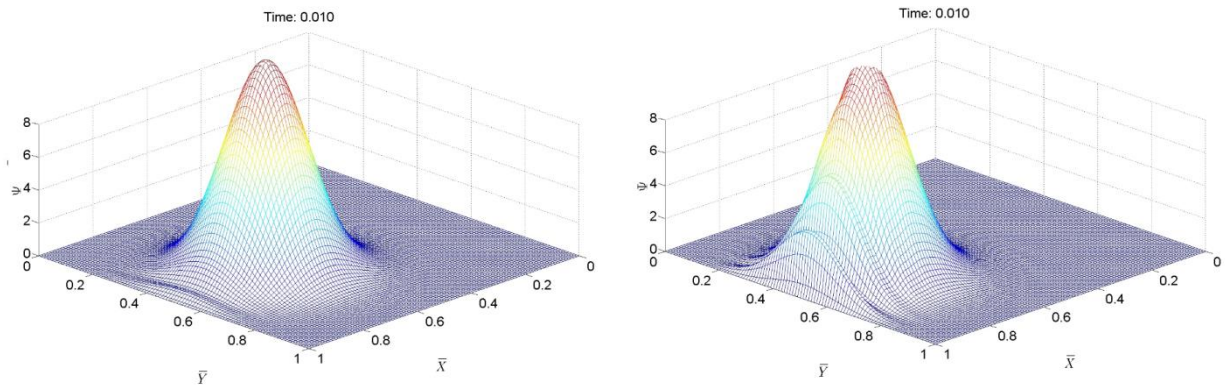
k=300



k=310



k=320



k=330 k=340

FIG 4.28. "Mesh" plots of a non-dispersive wave probability along X axis, in a grid without any voltage change, for different wavenumbers

With only a change of 80 in the range of the wavenumber, we were able to observe how the movement of the particle goes varying around 180 degrees in its direction, and that it goes changing more quickly than we have predicted. It can be intuited that the wave continues some periodicity in its movement related to the wavenumber. So there are some suggestions which seem to confirm the validity of this hypothesis. Despite of some facts that indicate us that perhaps this theory might be certain, we have not been able to obtain the direct relation between the wavenumber and the wave vector, so it cannot be taken for granted.

3) There is some kind of error given by MATLAB caused by a great value of the wavenumber. We are able neither to confirm nor to deny this affirmation, so it is only mentioned here as another possibility to consider.

4.8. WAVE-PARTICLE DUALITY

Perhaps since those times lost in the pages of the History when people started to ask themselves about the surrounding world, they were first intrigued about what were all the things done with, and not only the material ones. Different religions and philosophical tendencies tried to explain the essence of all that exists. It was in the Ancient Greece, the place of birth of the philosophy, where they started to argue about the nature of light. It is very interesting how people almost twenty five centuries ago have been so close to intuitively predict the nature of some phenomenon which started to be explained only a few hundred years ago. For example, Aristotle thought that the light was only some kind of disturbance in the material field, anticipating the wave behavior of the light; meanwhile, the atomists assured that all the things, including the light, were made by atoms, indivisible particles whose combination compose all the known things. Since those times, the most brilliant brains have discussed about the nature of light, but always defending the validity of only one condition and behavior of the light [21].

In the 19^{th} century, some experiments like the Young experiment (the one we try to reproduce numerically), and Huygens-Fresnel experiment (diffraction of the light), along with the discovery of the speed light by Maxwell, seemed to give a huge advantage to the wave theory. In was not until scientists tried to explain the photoelectric effect, with Planck constant being discovered a few years before, when they suggested the necessity of a light particle with a determined frequency that is absorbed by a single electron, exciting it and emitting it out of a

metal plate. Compton Effect, which consists in the increase of the wavelength (and therefore a decrease of the energy) of the light ray once it collides a free charged particle (generally an electron), also is better explained if it is assumed the light to be a corpuscle. Albert Einstein suggested to use what he called “light quanta” (later called photons), representing the wave-particle duality of the light. It can be said that the light follows the wave behavior during its movement, meanwhile during its interaction with other corpuscles, it can be described by a particle theory. Some years later, a French physicist Louis de Broglie suggested this principle of duality could not be exclusive for photons, but also should be valid for the rest of subatomic particles. The wave-like behavior of the matter had to be demonstrated. His hypothesis was experimentally proved using the diffraction of electrons in Davisson-Germer experiment and the scattering of the Helium atom, demonstrated by Stern and Estermann in 1930 [22].

4.9. DOUBLE SLIT EXPERIMENT [23]

A double slit experiment, also known as Young’s experiment after its inventor Thomas Young, is an important part of explanation and demonstration of the wave-like behavior of the light. Young tried to search some kind of similitudes between the light and the waves produced on the water surface after the perturbation. Two equal series of waves (that means those with the same frequency), with their origin close enough one to another, may overlap constructively, increasing the total amplitude along the lines where their individual amplitudes have their maximum (coinciding their phases), or they can also overlap destructively, decreasing the resulting height if a zero amplitude of one coincide with the maximum of the other (in other words, along the line where there phases are offset by 90 degrees within each other).

Now imagine that we have the same source of light focused on a barrier with two equal slits which are close enough for the light to hit them both. With this we can assure that the waves which pass through each slit have exactly the same frequency. The following image depicts the situation described above:

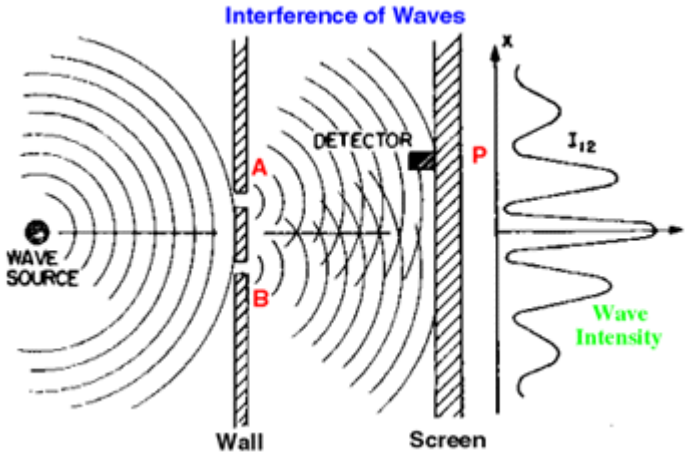


FIG 4.29. Schematic representation of the double slit experiment, with the depiction of the wave probability. Obtained from: https://glaukus.wordpress.com/2012/01/01/8/

The difference in the intensity is caused by the longer distances that the waves have to travel. The shortest way for both waves is exactly in the middle between two gaps, giving the brightest region; the two surrounding constructive lines are less brighten, been weaker as we move further from the center.

Attending to the accuracy of the simulation, the chosen barrier should be too high that the quantum effect away from the slits might be negligible (Ū=20000). The Gaussian wave packet is wide enough to hit both gaps, and the line of its movement is located exactly in the middle between both slits. The objective is to run a simulation where a non-dispersive Gaussian wave packet (with a chosen wavenumber equal to 100) crashes against a voltage barrier with two slits, and observe whether if the predicted phenomenon of destructive and constructive waves is produced. The measurement of the grid is $\bar{x}$=4 and $\bar{y}$=1. The position of the barrier and the initial wave is equal to one slit case. Here are also given the mesh plots, as well as the contour ones, taken for time intervals of Ŧ=0.002.

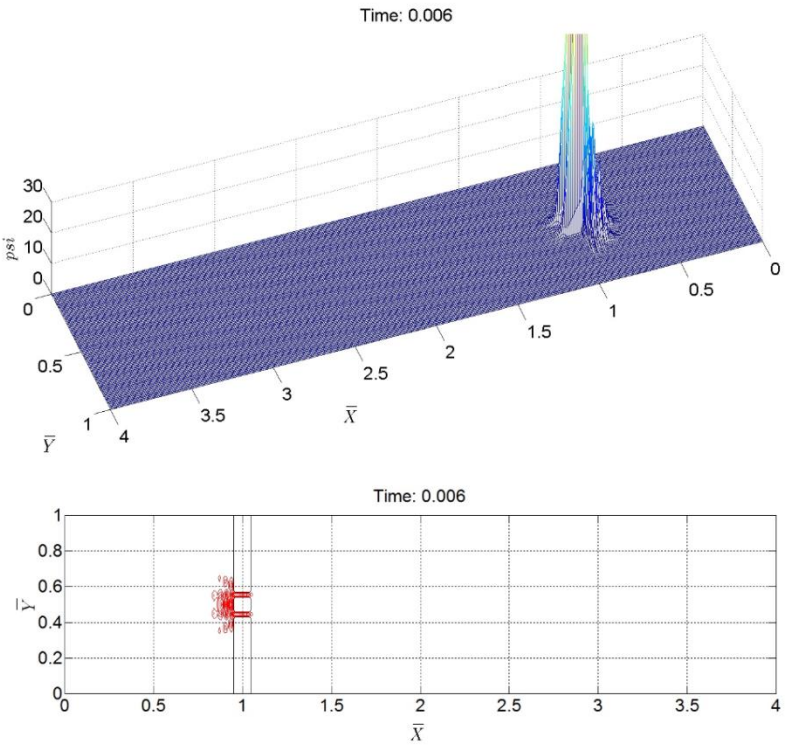


FIG 4.30. Ŧ=0.006. The incident wave has already crashed against the barrier and begins to enter the slits in a symmetrical way.

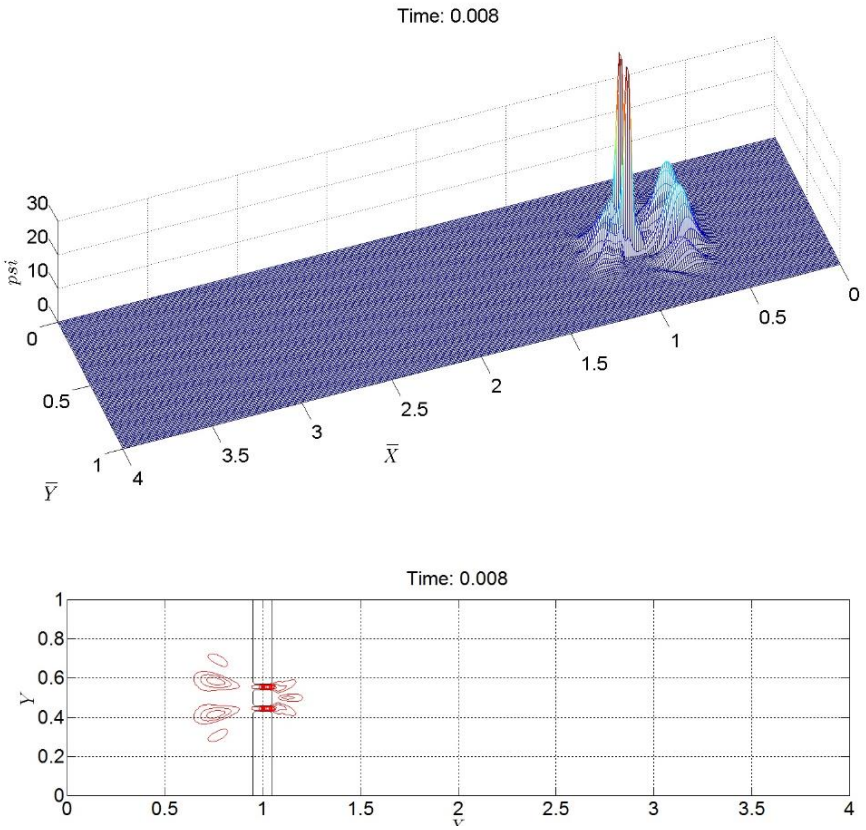


FIG 4.31. T=0.008. The splitting into three is slightly appreciated here.

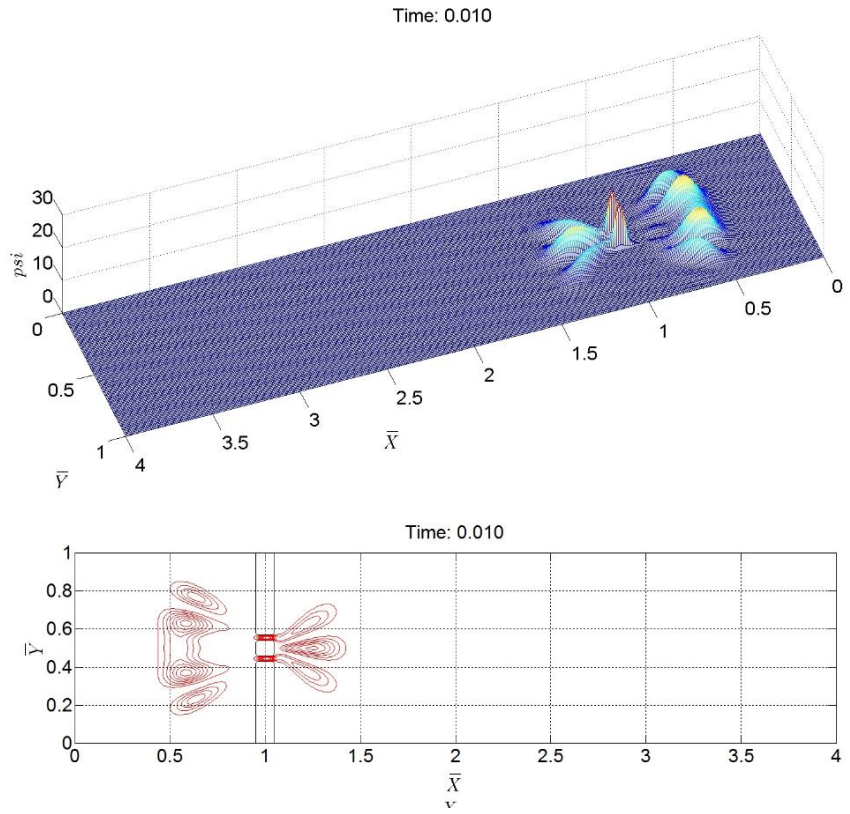


FIG 4.31. T=0.01. Apart from splitting into three, in the mesh plot there can be easily observed that the central part has its amplitude higher than the other two on the sides. Some part of the wave is still confined in the slits.

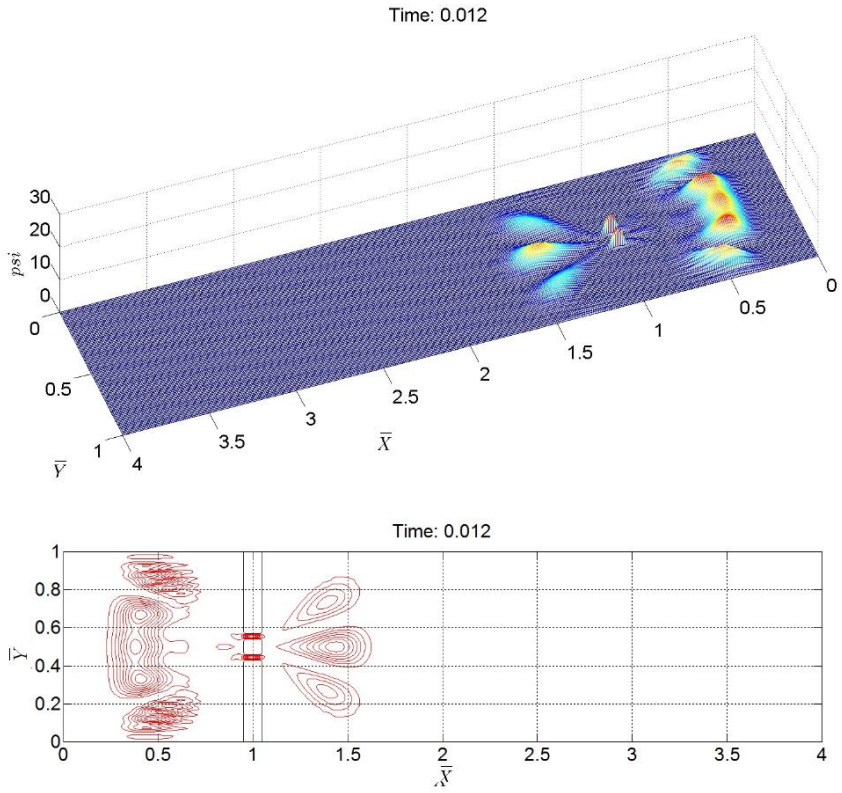


FIG 4.32. T=0.012

Last but not least, we add the graphic of the probability over the whole grid, looking if there were no significant changes in it.

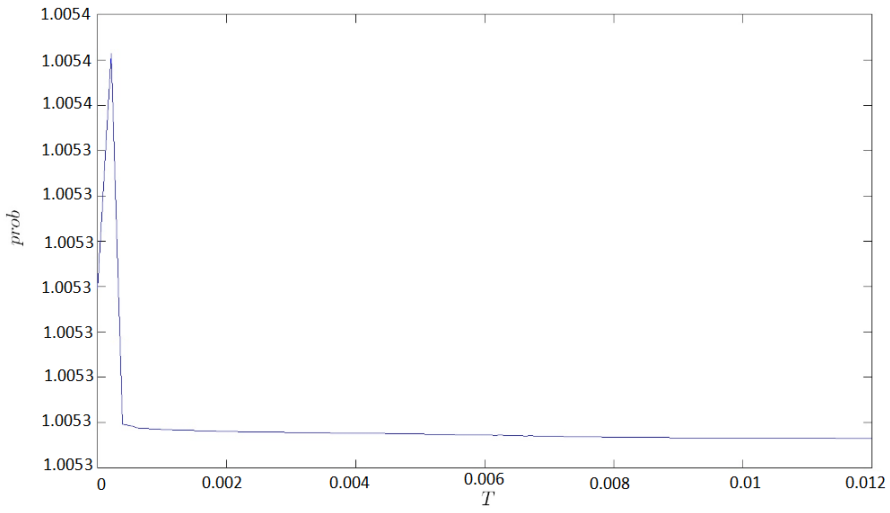


FIG 4.33. There is an insignificant variation at the beginning, probably caused by the crash against the voltage barrier.

Finally, it has been demonstrated that after passing a barrier which contains two slits, a wave probability of a particle described by Schrödinger equation in two dimensions splits into three parts, with all characteristics that demonstrate the wave behavior of a particle associated to this equation.

CHAPTER 5.CONCLUSIONS AND FUTURE WORKS

In the present work, we have developed a method of implementation of a numerical simulation of the Schrödinger equation in one and two dimensions using the program MATLAB as a chosen tool. Some cases have been studied, explaining several important and significant characteristics of the Schrödinger equation, such as the "quantum tunneling" and one and two slit barriers. Despite the Method of Lines, some others might be developed for the same purposes, for example the Leapfrog Method and the one using the Hamiltonian. The comparison between them ought to be interesting.

As guidance for some possible future works, a script for two particles in 1D could be written. In this case, every particle receives influences not only from an external field, but also from each other particle. Mathematically, the main difference between cases with one and more elements consists in the form of the Hamiltonian from the equation. If a general time dependent Schrödinger equation has the following expression (without applying the dimensionless form):

$$I\cdot\hbar\cdot\frac{\partial\Psi}{\partial t}=H\cdot\Psi$$

For only one particle (the number of dimensions is quite irrelevant, as here it is included in the Laplacian), the Hamiltonian operator has the following, already mentioned, form:

$$H=-\frac{\hbar^2}{2\cdot m}\Delta+V(r)$$

The Hamiltonian, by its definition, is an operator which corresponds to the total measurement of the energy of the system, including the sum of both the kinetic and the potential one. In case of two or more particles, the Hamiltonian is obtained by addition of the kinetic and the potential energy of each corpuscle (the potential energy is referred here as the one caused by an external field without the influence of other particles), plus that part of the potential energy which is originated by the interaction of particles taken two by two. For a general system consisting of N particles, the operator is as the following [24]:

$$H=\sum_{i=1}^{N}[-\frac{\hbar^2}{2\cdot m_i}\cdot\Delta_i+V_i(r_i)]+\frac{1}{2}\sum_{i\neq j}^{N}V_{ij}(r_{ij})$$

where:

$V_i(r_i)$=energy of the i particle in an external field, despising the potential caused by other particles

$V_{ij}(r_{ij})$=energy of mutual cooperation of two particles with numbers i and j.

Because of this interdependence of one in the behavior of the other, a simple simulation in one dimension with two wave probabilities cannot be used. If we try to describe two initial Gaussian wave packets, two dimensions ought to be utilized, because employing only one dimension of the following form:

FIG 4.34. A mistaken interpretation of the wave probability in one-dimensional case. Each particle has to be located in its own dimension.

In such way, we only denote one unique particle which may be located in any of the packets, not two material elements each one with its own initial Gaussian wave packet. To be able to describe two corpuscles, each one with its own characteristics (mass, initial position…), we require of two dimensions, one for each particle. In the case we increase the number of particles that interact in a unidimensional space, we grow as well the number of the dimensions used in the numerical simulation. And if the system is two-dimensional, we should operate twice as much. It is obvious that a matrix calculus in the form we have used it in the present work cannot be used here, so it is one of the numerous difficulties that the researchers who would do this simulation of "quantum billiard" might face.

There are also many works dedicated to study Schrödinger equation in cases where the prefixed Dirichlet Boundary Conditions are avoided [25][26]. In such simulations, the grid is usually unbounded.

As it was said in the introduction, Schrödinger equation is of great usefulness in non-relativistic cases. Nevertheless, for high speed systems, it provides huge mismatches, so Dirac equation is employed instead. Although the cases are quite different, some similitudes might be observed, as the major difference between bots consists in the form of the Hamiltonian, in the relativistic case called Dirac Hamiltonian. The comparison between the behavior and characteristics obtained from the simulations should be very interesting.

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